

PNNL Subsurface Science Scientific Focus Area
U.S. Department of Energy
Office of Biological and Environmental Research
Environmental Remediation Science Program

Role of Microenvironments and Transition Zones in Subsurface Reactive Contaminant Transport

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**WORK PROPOSAL REQUIREMENTS FOR OPERATING/EQUIPMENT
OBLIGATIONS AND COSTS**

Contractor Name Battelle Memorial Institute Pacific Northwest National Laboratory			Work Proposal No. 54737		Rev. No.		Date Prepared 01-30-08	
			FY 2011					
	FY 2009	FY 2010	Requested	Authorized	FY 2012	FY 2013	FY 2014	FY 2015
17. Staffing (in Staff Years)								
A. Scientific	20.1*	18.5*	18.0*		17.4*	16.8*		
B. Other Direct	1.1	0.9	0.8		0.8	0.8		
C. Total Direct	21.2	19.4	18.8		18.2	17.6		
18. Operating Expense (in Thousands)								
A. Total Obligations	6500	6500	6500		6500	6500		
B. Total Costs	6500	6500	6500		6500	6500		
19. Equipment (in Thousands)								
A. Obligations	365	578	500		500	500		
B. Costs	365	578	500		500	500		
20. Tasks or Milestones		Proposed Dollars				Proposed Schedule		Authorized Schedule
		FY 2009	FY 2010	FY 2011				
* Includes Post Doc FTEs (FY09 – 6.5; FY10 – 6.3; FY11 – 5.8; FY12 – 5.7; FY13 – 5.6)								

**U.S. DEPARTMENT OF ENERGY
OFFICE OF BIOLOGICAL AND ENVIRONMENTAL RESEARCH
ENVIRONMENTAL REMEDIATION SCIENCE PROGRAM
PROPOSAL**

1. TITLE OF PROPOSED PROJECT: Role of Microenvironments and Transition Zones in Subsurface Reactive Contaminant Transport

2. NUMBER OF SOLICITATION: N/A

3. NAME OF LABORATORY: Pacific Northwest National Laboratory

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15. REQUESTED FUNDING FOR EACH YEAR; TOTAL REQUEST:

	FY09	FY10	FY11	FY12	FY13	TOTAL
Expense	\$6,500,000	\$6,500,000	\$6,500,000	\$6,500,000	\$6,500,000	\$32,500,000
Capital	<u>\$ 365,000</u>	<u>\$ 578,000</u>	<u>\$ 500,000</u>	<u>\$ 500,000</u>	<u>\$ 500,000</u>	<u>\$ 2,443,000</u>
TOTAL	\$6,865,000	\$7,078,000	\$7,000,000	\$7,000,000	\$7,000,000	\$34,943,000

NOTE: See the attached budget pages for a detailed breakdown.

16. (a) USE OF HUMAN SUBJECTS IN PROPOSED PROJECT:

If activities involving human subjects are not planned at any time during the proposed project period, check "NO"; otherwise check "YES", provide the IRB Approval date and Assurance of Compliance Number and include all necessary information with the application.

() YES IRB APPROVAL DATE: _____

(X) NO ASSURANCE OF COMPLIANCE NUMBER: _____

(b) USE OF VERTEBRATE ANIMALS IN PROPOSED PROJECT:

If activities involving vertebrate animals are not planned at any time during this project, check "No"; otherwise check "YES" and provide the IACUC Approval date and Animal Welfare Assurance number and include all necessary information with the application.

() YES IACUC APPROVAL DATE: _____

(X) NO ANIMAL WELFARE ASSURANCE NUMBER: _____

17. SIGNATURE OF PI:

DATE:

18. SIGNATURE OF OFFICIAL:

DATE:

Subsurface Science Scientific Focus Area
U.S. Department of Energy
Office of Biological and Environmental Research of the Office of Science
Environmental Remediation Science Program

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Abstract

The PNNL Scientific Focus Area (SFA) will resolve critical Hanford and basic subsurface science issues through integrated, multi-disciplinary, science-theme focused research on the role of microenvironments and transition zones in the reactive transport of technetium (Tc), uranium (U), and plutonium (Pu). The overall ten-year goals of the SFA are to develop: i.) an integrated conceptual model for microbial ecology in the Hanford subsurface and its influence on contaminant migration, ii.) a fundamental understanding of chemical reaction, biotransformation, and physical transport processes in microenvironments and transition zones, and iii.) quantitative biogeochemical reactive transport models for Tc, U, and Pu that integrate multi-process coupling at different spatial scales for field-scale application. The SFA will build on established areas of PNNL expertise in geochemistry, microbiology, and multi-scale modeling. The SFA consists of eleven projects involving twelve external collaborators that fall into the following science categories: i.) microbial ecology, ii.) molecular scale mechanisms, iii.) pore-scale coupled processes, iv.) reactive transport science, v.) multi-scale reactive transport models, and vi.) in-situ structures and reactive transport properties. Cohesiveness and integration will be achieved by focus on four SFA hypotheses and Hanford-relevant contaminant scenarios to enhance information upscaling, resolution of broader science issues, and Hanford impact. The SFA relies strongly on the Environmental Molecular Sciences Laboratory (EMSL) for fundamental science capabilities and the Hanford Integrated Field Challenge (IFC) site as an essential location for samples and opportunities for field scale research.

Executive Summary

The PNNL Scientific Focus Area (SFA) will resolve critical Hanford and basic subsurface science issues through integrated, multi-disciplinary, science-theme focused research on the role of microenvironments and transition zones in the reactive transport of technetium (Tc), uranium (U), and plutonium (Pu). Microenvironments are small domains within larger ones that exert a disproportionate influence on subsurface contaminant migration. They may be internal fractures or microbiologic niches within porous media lithic fragments; grain coatings, bio-films, or micro-colonies on larger mineral particles; or compact silt/clay stringers in gravel-dominated subsurface sediments. Transition zones are field scale features where chemical, physical, or microbiologic properties change dramatically over relatively short distances (e.g., ≤ 1 m). They exhibit steep, transport-controlled gradients of system-controlling chemical species such as O_2 , H^+ , or organic carbon. Microenvironments and transition zones frequently dominate subsurface contaminant reactivity, with strong effects resulting from the coupling of chemical reaction, physical transport (advection, diffusion), and microbiologic processes. Past EMSP and NABIR research has documented the importance of these zones at the Hanford site.

The overall ten-year goals of the SFA are to develop: i.) an integrated conceptual model for microbial ecology in the Hanford subsurface and its influence on contaminant migration, ii.) a fundamental understanding of chemical reaction, biotransformation, and physical transport processes in microenvironments and transition zones, and iii.) quantitative biogeochemical reactive transport models for Tc, U, and Pu that integrate multi-process coupling at different spatial scales for field-scale application. Targeted contaminant chemical reaction and biotransformation processes include heterogeneous/biologic electron transfer, precipitation and dissolution, and surface complexation. The SFA will emphasize lab-based, coupled computational and experimental research using relevant physical/biologic models, and sediments and microbial isolates from various Hanford settings to explore molecular, microscopic, and macroscopic processes underlying field-scale contaminant migration. It will also pursue the refinement of geophysical techniques to define, characterize, and map spatial structures and reactive transport properties of microenvironments and transition zones in the field. The SFA will partner with the PNNL Environmental Molecular Sciences Laboratory (EMSL) to develop molecular understandings of key processes, and the Hanford Integrated Field Challenge (IFC) for access to, and samples from subsurface environments where these zones exist and are important.

The SFA will build on established areas of PNNL expertise in geochemistry, microbiology, and multi-scale modeling. Eleven individual, but highly collaborative research projects will focus on different scales, coupled processes, and/or contaminants; each will be managed by a PNNL-ERSD investigator of significant accomplishment and appropriate expertise. The projects fall in the following science categories: i.) microbial ecology, ii.) molecular scale mechanisms, iii.) pore-scale coupled processes, iv.) reactive transport science, v.) multi-scale reactive transport models, and vi.) in-situ structures and reactive transport properties. An additional small project will also be established to mentor a promising new or young investigator. The PNNL team will be supplemented with 12 external, PNNL-supported investigators (lab, university) with needed complementary expertise. Cohesiveness and integration will be achieved by focus on SFA hypotheses formulated to enhance information upscaling, resolution of broader science issues, and Hanford impact. The overall SFA science program will be managed by two PNNL Chief Scientists who collectively have more than 40 years experience as BER PI's in subsurface biogeochemistry and contaminant fate and transport.

Narrative

Concept

The PNNL SFA will focus on Hanford subsurface science issues and will closely align with the ERSD-funded, PNNL Integrated Field Challenge (IFC) which is being performed at the 300 A uranium plume (<http://ifchanford.pnl.gov/>). PNNL senior scientists have considered the ERSD strategic plan, PNNL institutional goals, unique facilities and staff expertise, and Hanford's most significant subsurface science challenges to identify a long-term scientific theme for the PNNL-SFA. This theme focuses on the importance of microenvironments and transition zones upon reactive contaminant transport with emphasis on the Hanford Site. Through our long and active association with the Hanford Site, the PNNL team has come to recognize that these environments are a fundamental, yet poorly understood subsurface feature that merit a sizable, integrated, multidisciplinary research effort with high potential scientific impact. While the SFA focuses on Hanford, the research will be sufficiently fundamental in nature that it will be broadly applicable to DOE and other contaminated sites nationwide.

The definition of microenvironment is conditional to the overall scale of observation, and to personal perspectives. We define "microenvironments" as submicron to meter scale domains that exert disproportionate influence on the water chemistry of larger vadose or aquifer zones because of integrated microbial, geochemical, and hydrophysical processes that occur at dissimilar or accelerated rates within them. If the observation scale is on the order of a millimeter, then included microenvironments may exist on the scale of nanometers to microns. In contrast, if the observation scale is tens of meters, then a microenvironment could be on the scale of meters, and so on. Microenvironments and transition zones frequently dominate subsurface contaminant reactivity, with strong effects resulting from the coupling of chemical reaction, physical transport (advection, diffusion), and microbiologic processes (Jakobsen, 2007; Li et al., 2007; Liedl and Ptak, 2003; Meile and Tuncay, 2006; Thullner et al., 2007). Understanding the function of these zones and modeling their behavior is a forefront issue in subsurface science (Steeffel et al., 2005). Moreover, the presence of microenvironments that chemically react with (e.g., adsorption or precipitation) or hydrophysically retard contaminants can exert a huge impact on the ability to successfully remediate contaminated subsurface zones (Haggerty and Gorelick, 1995; Mackay and Cherry, 1989).

Subsurface microenvironments are often associated with centimeter to meter scale regions of porous media where advective water movement is slow, and connection to the advective domain occurs through diffusive mass transfer (Watson and Baxter, 2007). Biotic microenvironments may consist of: i.) thin

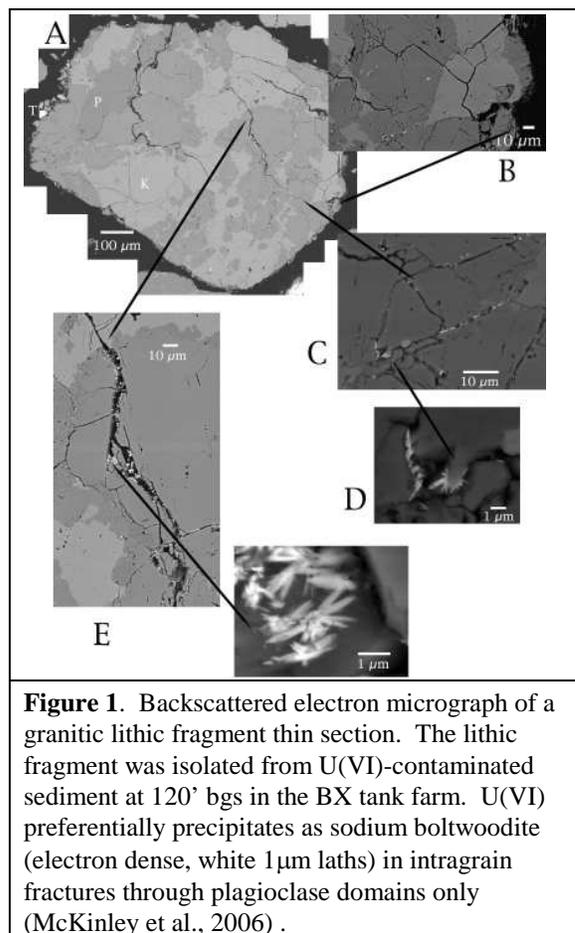


Figure 1. Backscattered electron micrograph of a granitic lithic fragment thin section. The lithic fragment was isolated from U(VI)-contaminated sediment at 120' bgs in the BX tank farm. U(VI) preferentially precipitates as sodium boltwoodite (electron dense, white 1 μm laths) in intragrain fractures through plagioclase domains only (McKinley et al., 2006).

(mm) biofilms or small microcolonies where pH, water composition, metal ion concentrations, and organism types and activities vary spatially with respect to mineral surfaces; ii.) a sub-pore scale

microniche where microorganisms deplete O₂ leading to localized anoxic conditions in an otherwise oxidized groundwater flow domain; or iii.) a sub-micron scale interface where mineral-bound microorganisms alter near-surface pH and enzymatically oxidize structural Fe(II) or Mn(II) to produce reactive, Fe(III)- or Mn(IV)-oxide precipitates. Microenvironments where abiotic processes predominate due to limited microbial energy sources include various restricted physicochemical settings in intra-grain regions of mineral matter (e.g., Figure 1), associated mineral aggregates, or geologically derived sediment structures. In these environments, pore fluids evolve to different chemical end states than the bulk fluid due to: i.) enhanced residence times influencing the progress of kinetically controlled reactions, ii.) diffusional limitations coupled with exposure to mineral surfaces that preferentially dissolve or precipitate, or that are enriched in surface sites of different character, function, and reactivity, and iii.)



Figure 2. Silt-textured stringers containing phyllosilicates with high cation exchange capacity and water retention properties are common features of Hanford subsurface sediments. These are often associated with discontinuous zones of calcium carbonate (caliche) precipitation because of local effects on water migration.

local water content variations resulting from lithologic and hydraulic non-uniformities. These sites include centimeter- to meter-scale silt layers of phyllosilicates (e.g., Figure 2) sometimes with weathering-product, micro-precipitates of Fe(III) oxides; millimeter sized internal fractures and differentially weathered zones in lithic fragments of different provenance (Figure 3); and micron and nanometer-sized pores of varying connectivity in particle coatings, carbonate cements, and phyllosilicate aggregates.

Transition zones are field scale features through which chemical, physical, or microbiologic properties change dramatically over relatively short distances (e.g., ≤ 1 m) to influence, or in response to, contaminant migration. These zones may exhibit different physical structures depending on depositional environment and geology, and are characterized by steep, transport-controlled gradients of system-controlling chemical species such as O₂, H⁺, or organic carbon. Various examples of these features occur at Hanford: i.) pH neutralization fronts beneath sites that have leaked acidic or basic wastes; ii.) the capillary fringe boundary between the vadose zone and the unconfined, suprabasalt aquifer; iii.) the Hanford-Ringold contact in the unconfined aquifer; iv.) oxic-anoxic facies below the 300 A water table in the Ringold Formation (e.g., Figure 4); and v.) the river-shore environment where groundwaters and river waters mix and discharge through the hyporheic zone to the Columbia River. Contaminant stability, speciation, and reactivity may vary

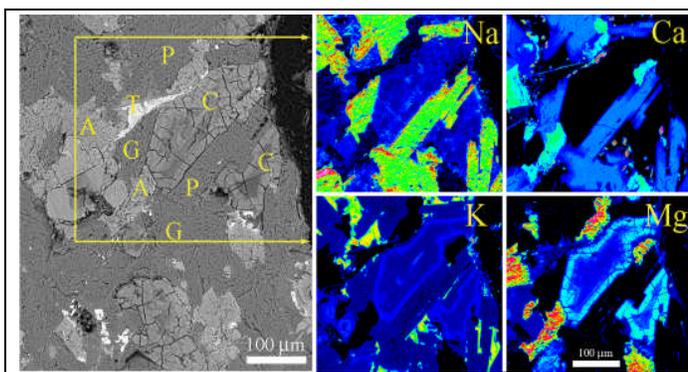


Figure 3. Unique microenvironments are found in certain basalt fragments where glass (G) has weathered to saponitic (Fe-containing) clay (C). The saponite zones are clearly identified in this lithic fragment thin section imaged by backscattered electron microscopy and electron microprobe by zonation in Mg composition. These zones interact with pore fluids through diffusive exchange and are the primary locations for radiocesium adsorption such as ⁹⁰Sr (McKinley et al., 2007b).

markedly across such transition zones while remaining relatively stable for significant transport distances both above and downgradient of these more active locations. Thus, they are focal points for biogeochemical and hydrodynamic change that must be understood for system prediction. Transition zones may have dynamic spatial and temporal characters if influenced by changes in temperature, water content or pore space saturation, or chemical composition. These dynamics are especially important along the Hanford Reach where the Columbia River-groundwater system is subject to 1-3 meter changes in river flow stage on seasonal timeframes and even daily as a consequence of water flow management via dams. These river stage effects force marked changes in associated groundwater compositions, temperature, and dissolved carbon/nutrient levels.

A common aspect of both microenvironments and transition zones is that their overall behavior is strongly influenced by the coupling of molecular, microscopic, and macroscopic geochemical, microbiologic, and physical transport processes. Moreover, their properties, associated processes, and in-situ chemical contributions must be understood at various spatial scales to accurately forecast the long term, field behavior of high-risk contaminants at Hanford as will be briefly described below. It is these complex linkages, interdependencies, and their profound impact on reactive contaminant transport over a range of spatial scales that are the focus of the PNNL ERSD SFA. PNNL investigators and their collaborators have actively published on various subject areas related to this science theme and are internationally recognized (see **Biographical Sketches**). The SFA will serve to align these accomplished PNNL investigators and talented new staff, complemented by external experts, along a common multi-disciplinary theme for higher scientific impact and enhanced contributions to Hanford contaminant fate and transport knowledge needs. Moreover, this SFA is in direct support of DOE-ERSD's mission to "advance our understanding of the fundamental biological, chemical, and physical processes that control contaminant behavior in the environment in ways that help solve DOE's intractable problems in environmental remediation and stewardship."

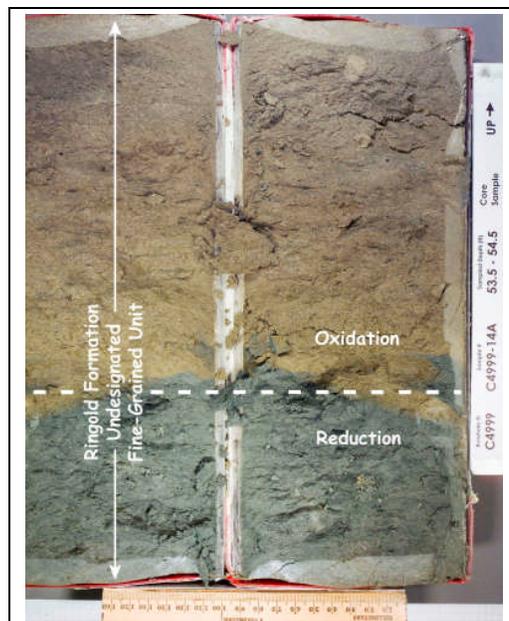


Figure 4. Redox boundary in 300 A Ringold sediments about 2.5 m below the Hanford-Ringold contact. The boundary represents a point where oxygen and other terminal electron acceptors have been consumed by microbiologic respiration. Residual organic matter in the sediments is believed to be the electron donor for this process. This reducing zone appears to collect contaminant U(VI) that migrates from above under conditions of high groundwater U (Williams et al., 2007).

Background and Justification

The PNNL SFA is focused on fundamental Hanford subsurface science needs. However, the Hanford Site is one of the world's largest, most complex, and costly environmental remediation projects. Consequently, diverse and often conflicting views exist on all issues including science needs. There are many players at the site including the PNNL which has been an active player in Hanford research since 1964, and various remediation contractors that come and go on approximate 5 year time frames. PNNL is arguably the dominant holder of Hanford-site science expertise because of its long and sustained engagement, and the institutional priority it has placed on resolving both fundamental and applied

science issues at the site. PNNL's role in Hanford science and technology was recently reviewed by the National Research Council (NRC, 2001).

Science needs and gaps for Hanford are evaluated periodically by different groups and teams, often with different objectives and biases, but PNNL is generally an important participant. Recent, example assessments of this sort include: Cantrell et al. (2007); Mann et al. (2007); Zachara et al. (2007c); Zachara et al. (2007a). These identify the "high inventory" contaminants U, ^{99}Tc , ^{129}I , Cr, and CCl_4 as being risk drivers because of their environmental mobility and persistence; and $^{239,240,241}\text{Pu}$, ^{137}Cs , and ^{90}Sr as problematic because of relatively low mobility but high radioactive toxicity. All credible data analyses for Hanford admit to the poor existing capability to predict subsurface contaminant migration because of: i.) insufficient understanding of controlling processes (hydrology and geochemistry primarily), and lack of robust process-level models and parameters to describe them; ii.) a historic and continued lack of consideration of any and all kinetic processes; iii.) inadequate characterizations of subsurface properties, structures, and features over the large-scale domains of interest; and iv.) lack of modeling approaches to quantitatively deal with substantial heterogeneities in chemical and physical properties at different scales (See Figures 5 and 6). The SFA recognizes these inadequacies and seeks to resolve key issues that will substantially advance the field of fundamental subsurface science.

Underappreciated by the Hanford community is the important role of subsurface microorganisms in transforming contaminant speciation; modifying solubility; precipitating or dissolving mineral phases; consuming/assimilating carbon, oxygen, and other electron donors; and modifying contaminant transport through other means. These phenomena have been a long-term focus of ERSD/OBER research which has developed the world's preeminent understanding of the microbiologic transformations of Tc, U, Cr, and Pu. Such transformations could be highly significant to long-term stewardship, but have generally been ignored in Hanford "performance assessments" as they represent "one more thing to look at" for those seeking cost-incentives rather than effective and informed, long term clean-up. Selected subsurface microbiology investigations were performed at Hanford, mainly in the western central plateau, in the early 1990's by ERSD predecessor programs (Fredrickson et al., 1995; Kieft et al., 1995; McKinley et al., 1997). Little additional research on Hanford microbial ecology and subsurface biogeochemical processes has been performed since that date except for an ERSD/LBNL biostimulation experiment for chromate reduction in Hanford's 100 A (Hazen et al., 2006); characterization of microorganisms (Figure 7) in a chemically- and radiologically-extreme high level waste plume (Fredrickson et al., 2004a); and a study of the biogeochemistry of Columbia River hyporheic zone sediments (Moser et al., 2003). This limited information on Hanford subsurface microbiology, especially in sensitive near-shore regions along the Columbia River corridor, has motivated the SFA to place significant research emphasis on identifying the nature and function, and contaminant transformation potential of Hanford microbes, and models to describe their behaviors at different levels.

Our SFA science theme selection on microenvironments and transition zones derives from numerous



Figure 5. Cataclysmic flood deposits of the Hanford formation exposed in Hanford's central plateau where major vadose zone contamination exists. Micro-environments and zones of different scale and lateral connectivity are ubiquitous, leading to large challenges in predicting water migration and reactive contaminant behavior.

observations made by our ERSD science team members at different Hanford sites, and other relevant locations. These include observations regarding the speciation, location, and mass transfer kinetics of various Hanford contaminants sorbed in distinct microenvironments (Arai et al., 2007; Catalano et al., 2006; Liu et al., 2003; Liu et al., 2004b; McKinley, 2001; McKinley et al., 2006; McKinley et al., 2007a; McKinley et al., 2007b); modeling chemical and

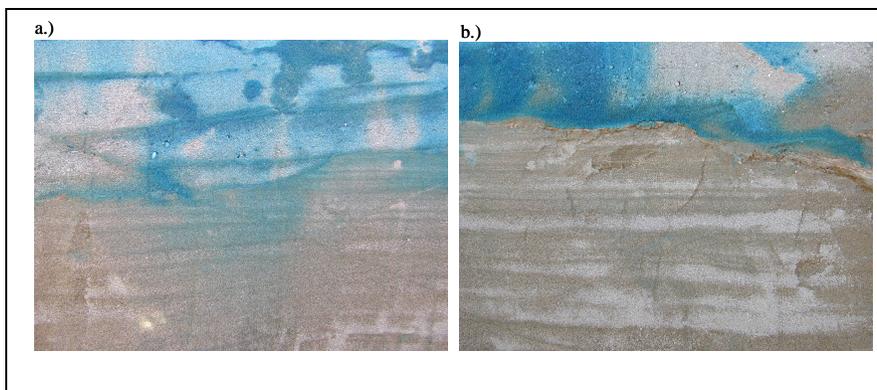


Figure 6. In-situ dye-tracer experiment performed at the BER/EMSP clastic dike field research site. Each panel represents a zone that is 1.5 m (wide) x 1 m (high). Zones of most intense blue represent those of higher water content, or those where tracer dilution by native waters was minimal. Water migration paths and dye accumulation show extremely complex behavior that sometimes correlates with evident stratigraphic and structural features (Ward, 2006).

transport behaviors at different scales (Liu et al., 2008; Liu et al., 2006b; Qafoku et al., 2005; Roden and Scheibe, 2005; Scheibe, 2004; Tartakovsky et al., 2007b), and defining the important roles of various heterogeneity forms on field scale water migration and hydrophysical retardation (Stewart et al., 2006; Ward, 2006; Ward, 2007; Ward et al., 2006). Additionally, with support from ERSD through the Hanford linkage project, our ERSD research team has maintained a bibliography of all Hanford-relevant publications in geochemistry, hydrology, environmental microbiology, and remediation technologies since 1997 (over 250 publications). This bibliography is used to inform site contractors, to monitor resolution of key science and technology issues, and to identify emerging or key remaining Hanford science questions. This bibliography was drawn upon during SFA development. Our extended research group also edited the November 2007 issue of the Vadose Zone Journal that was dedicated to the Hanford Site, and strongly contributed to its scientific proceedings. These activities and others have provided our ERSD research team with unique science perspectives on the Hanford Site that led to the conceptualization of our theme.

The PNNL SFA will focus on the high risk, polyvalent, radionuclide contaminants U, Tc, and Pu. Each of these contaminants can adopt multiple valence states in the environment depending on the redox potential, concentrations of microbial electron donors and acceptors, and the presence and types of agents (microorganisms, solutes, and mineral surfaces) that can facilitate electron transfer reactions. The first two radionuclides (U and ⁹⁹Tc) are soluble in their oxidized states, poorly soluble and therefore

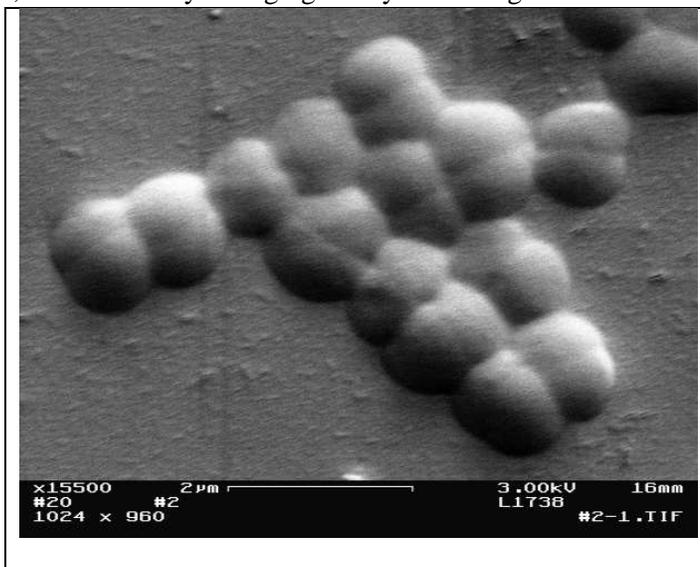


Figure 7. A broad selection of microorganisms was found to reside within an incredibly harsh vadose zone plume of high level waste beneath the S-SX tank farm (Fredrickson et al., 2004a). Sediments within the plume had experienced extremely high levels of salt, pH, radiation, chemical contamination, and temperature, and low moisture content. The image shows a new strain of the radiation-resistant and desiccation-tolerant bacterium *Deinococcus radiodurans* that was isolated from the plume.

relatively immobile in their reduced states, were released to the vadose zone at high inventory ($U = 202,703 \text{ kg}$ and $^{99}\text{Tc} = 1390 \text{ Ci}$), and have formed groundwater plumes in multiple locations at Hanford that are either currently or are projected to migrate to the Columbia River (Hartman et al., 2007). Additional groundwater plumes of these solutes are forecast for the future as deep vadose zone contamination continues to discharge to groundwater. Given the water quality criteria for U (MCL = 30 ppb), the in-ground inventory could yield the sizable problem of $2 \times 10^{15} \text{ L}$ of contaminated groundwater (@ 100 ppb). Technetium poses extreme environmental risk because of high subsurface mobility under oxidizing conditions, a low regulated concentration in water (e.g., MCL $<10^{-9} \text{ mol/L}$), long half-life ($t^{1/2} = 2.13 \times 10^5 \text{ y}$), and often “point-source” mode of release. Plutonium (Pu) is a problematic contaminant because of high public concern, health implications, and sizeable in-ground inventory (~400 kg). Although it is highly insoluble and immobile as a precipitate in its most common environmental state [Pu(IV)], it can be mobilized by strong acid, complexation by organic ligands, formation of or binding to mobile colloids, and reduction to more soluble valence states. It has moved deep (>30m) into the vadose zone in several Hanford locations (beneath Hanford’s Z-cribs) for reasons that are poorly understood, posing difficult questions for future disposition. DOE seeks markedly improved methods and scientific understanding to predict the future behavior of these three radionuclides as a basis for selecting sound, in-ground management procedures such as monitored natural attenuation and/or more aggressive remedial actions. Members of the SFA team have actively published on the (bio)geochemical behavior of these contaminants and geochemical/transport modeling of their behavior (see **Biographical Sketches**), and recently completed a definitive review of the inventory, distribution, geochemistry, and scientific issues regarding U subsurface migration at Hanford (Zachara et al., 2007a). Comparable review and synthesis efforts are underway for Tc, and planned for Pu. Thus, the team is, or soon will be, well informed on current science issues associated with these three key Hanford contaminants.

The geologic, mineralogic, and geochemical characteristics of Hanford Site sediments are conducive to microenvironment and transition zone formation. Upper vadose zone sediments in the 200 A plateau, and vadose zone and upper unconfined aquifer sediments in the Columbia River corridor (e.g., the 300 A) are comprised of the relatively unweathered, Pleistocene-age Hanford formation. These sediments are dominated by basaltic and granitic lithic fragments in various states of comminution (Figure 8a), with interspersed silt and clay-sized detrital phyllosilicates (chlorites, and ferruginous biotites). They contain significant total Fe (~8%), of which 53% or more exists in the reactive ferrous state (Figure 9b).

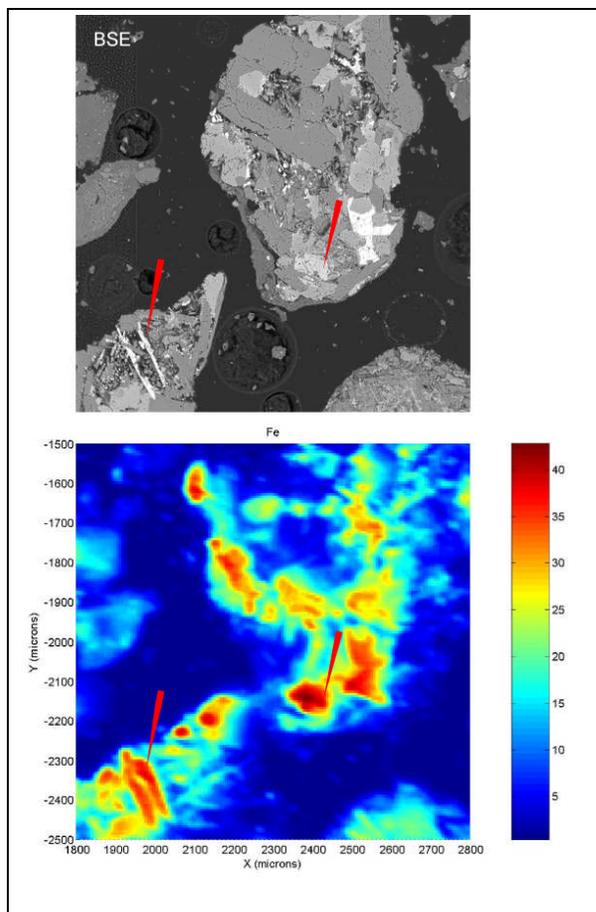


Figure 8. Backscattered electron micrograph of a sediment thin section displaying basaltic lithic fragments (a). X-ray fluorescence microprobe analyses for Fe performed at the Advanced Photon Source show regions of Fe localization in the particles (b). The crystallites that contain Fe are primarily magnetite, ilmenite, and pyroxenes, and are speculated to be intra-grain locations of redox reactivity that may consume oxygen or reduce contaminants (Results in publication).

The lithic fragments contain fractures, microporosity, parting along grain interfaces (Figure 8a), and display significant intraparticle Fe (Figure 8b) in the form of the Fe(II)-containing mineral phases magnetite, titanomagnetite, augite, and clinocllore. A magnetic fines fraction exists containing magnetite, Fe(III) oxides, augite, and chlorite (Figure 9c). In the absence of surface passivation, these ferrous minerals should be active polyvalent metal reductants [e.g., (Lloyd et al., 2000)], and evidence gathered to date strongly suggests that the interiors of Hanford lithic fragments (or possibly grain interfaces of ferrous minerals) are reducing microenvironments, especially if oxygen is scavenged by associated oxygen-consuming mineral reaction or microbial respiration. Microenvironments in extended phyllosilicate aggregates and caliche stringers are equally prevalent and present different geochemical implications.

The older, Pliocene-age Ringold Formation lies below the Hanford formation, and comprises the deep vadose zone and unconfined aquifer in the 200 A, and the deeper unconfined aquifer in the Columbia River corridor. Ringold sediments are more weathered, and contain visible Fe(III) oxides (e.g., Figure 4, upper half). In fine-grained Ringold facies, apparent oxic-anoxic transition zones are observed (Figure 4; these are as yet uncharacterized and unstudied) that are hypothesized to result from microbiologically-driven, terminal electron acceptor consumption [e.g., O₂, NO₃, Mn(III/IV), Fe(III)] in transport-limited regions leading to low redox potential Fe(III) oxide reduction and dissolution. This particular zone exists only 1-2 m below the 300 A uranium plume in the more permeable Hanford formation, and presumptive evidence (Williams et al., 2007) suggests that it is a zone of U collection through biologic and/or heterogeneous reduction.

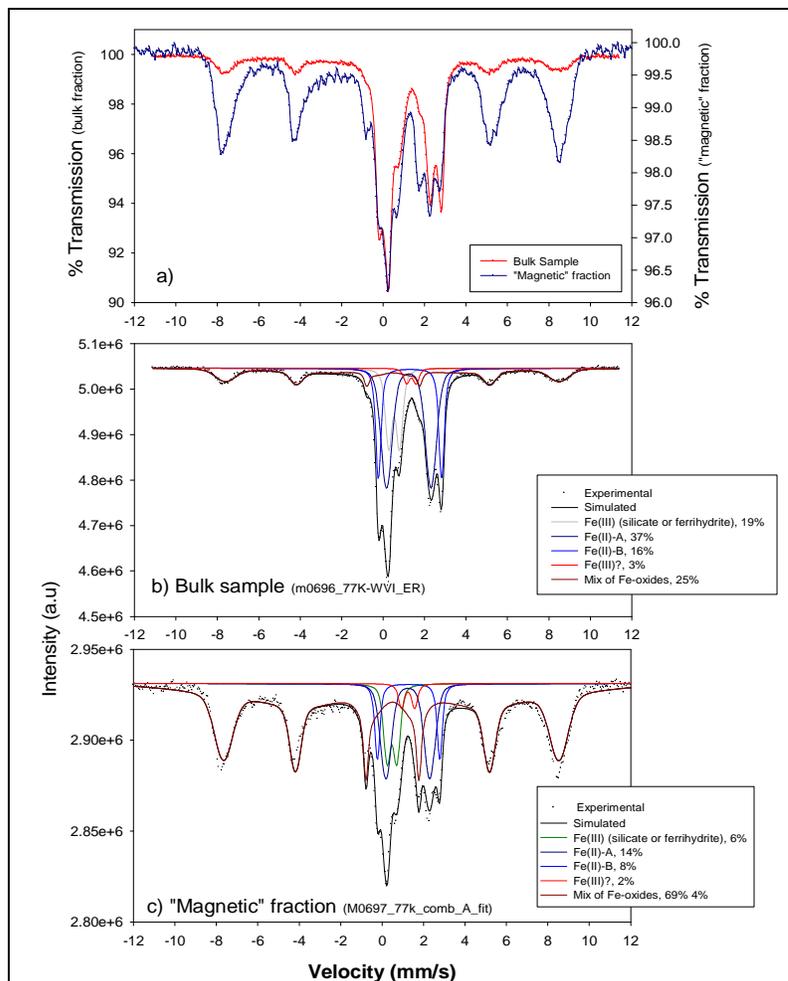


Figure 9. Transmission Mossbauer spectroscopy (77K) of bulk U(VI)-containing 300 A capillary fringe sediment (SPP2-18) from Hanford, and magnetic particles isolated from the sediment. Measurements performed in EMSL's Mossbauer facility. Results show that 53% of the Fe in the bulk sediment is Fe(II) existing in multiple environments designated for simplicity here as A and B (b). The finer grained magnetic fraction (c) contains similar Fe(II) environments (A&B), as well as a mass dominant mix of Fe-oxides (69%) believed to be partially weathered magnetite (Results in publication).

Research Program

The text that follows describes an approximate 5 to 10 year research plan for the PNNL SFA. In keeping with ERSD's request, the research program is described in relatively high-level terms, and has not been prepared as a proposal. However, we have tried to provide enough detail so that fundamental science aspects and potential accomplishments of the research are evident.

Hypotheses

The overall ten-year goals of the SFA are to develop: i.) an integrated conceptual model for microbial ecology in the Hanford subsurface and its influence on contaminant migration; ii.) a fundamental understanding of chemical reaction, biotransformation, and physical transport processes in microenvironments and transition zones, and iii.) quantitative biogeochemical reactive transport models for Tc, U, and Pu that integrate multi-process coupling at different spatial scales for field-scale application.

The following global hypotheses will guide research in the first 5 y of the SFA.

- Microorganism species richness and equitability will increase in groundwaters near the Columbia River. The functional properties and redundancy of microbial communities will be determined by local microscale geological, chemical and hydrological conditions that are subject to seasonal variation. Resident microbial communities will coincidentally catalyze biogeochemical transformations of U, Tc, or Pu and/or modify aqueous, mineralogic, or surface chemical properties to affect contaminant migration.
- Hanford subsurface microenvironments and transition zones will be dominant regions of contaminant reaction. Reductive valence transformations (heterogeneous and biologic) of Pu, Tc, and U will occur in microenvironments where: oxygen is consumed by microbiologic respiration; microorganisms populate their cell envelope with redox-active biomolecules; and ubiquitous ferrous containing mineral solids are exposed for dissolution and reaction. Oxidation reactions will be retarded in these zones of higher intrinsic oxygen consumption as compared to advectively dominated ones where oxygen is more rapidly replenished. Contaminant precipitation reactions will also be promoted in these domains as a result of heterogeneous nucleation and local pore water compositions that differ from bulk.
- Diffusion-controlled mass transfer will aid in the establishment and maintenance of microenvironments and transition zones in Hanford subsurface sediments. Restricted solute mass transfer will occur at multiple scales and will cause disequilibrium between advectively transported waters and diffusion controlled fluids in nano- to micro-domain pores, and interiors of grains, grain aggregates, microbial cell aggregates, and fine-grained sediment bodies. Mass transfer will regulate solute, nutrient, reactant, and contaminant fluxes to and from sites of biologic and geochemical reaction, and consequently the rates and extent of these important processes.
- The dominant processes within microenvironments and transition zones will vary with scale from microns to meters. At the smallest scale, heterogeneities in mineral and biological structures, and

chemical composition/functionality will create nano-sites of disproportionate molecular reactivity that dominate the (bio)geochemical behavior of larger microscopic reaction domains. At the largest scale, geologically structured heterogeneities in grain size distribution, permeability/porosity/tortuosity, and mineralogy and natural organic matter, will control linkages between abiotic (transport, geochemistry) and biotic processes at the macroscopic scale to create localized zones of reaction that dominate field scale contaminant migration.

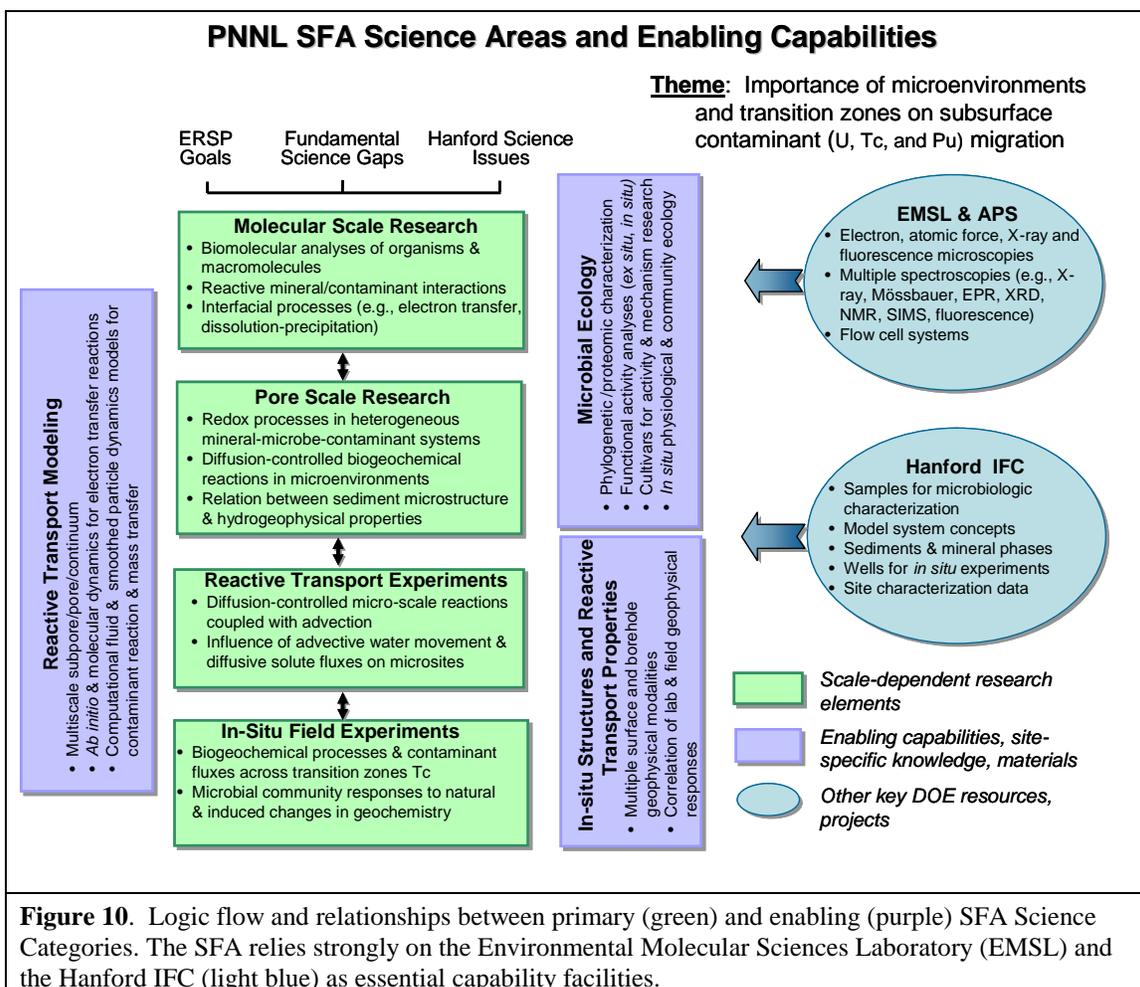
General Scientific Content and Approach

The SFA will emphasize scientific issues identified or implied to be important by field observations at Hanford and other DOE sites that will be explored at different and appropriate scales through fundamental research in the laboratory, and at selected field sites. SFA research will emphasize lab-based experimentation with model systems and field samples; exploring molecular, microscopic, and macroscopic mechanisms and phenomena underlying coupled microbiologic, geochemical, and hydrogeophysical behavior in the field. The SFA will also engage in select field studies coordinated with the PNNL Hanford IFC to provide a robust understanding of the contributions of microenvironments and transition zones to field scale behavior. To accomplish this, the SFA will develop mechanistic understandings of the functioning of microenvironments and transition zones and hydrogeophysical means to characterize their spatial and temporal properties and extent, while the IFC site will provide access to subsurface environments where these zones exist and are significant to contaminant transport and/or microbial ecology and biogeochemistry. Selected smaller field sites of opportunity in the 200 A, and along the Columbia River corridor will also be used as appropriate and necessary. The close linkage of PNNL research to the Hanford Site, and our historic success in providing fundamental scientific solutions for Hanford's complex subsurface contaminant migration issues from individual NABIR/EMSP projects supports our contention that the SFA will have a major positive scientific impact at Hanford. Because of the generic and timely significance of our theme, progress toward ERSP-specific goals will also yield high quality results for publication that will be in demand by the scientific community and that will advance the state of science.

The PNNL SFA includes primary (green) and enabling (purple) research areas with integration and overall logic flow as shown generally in Figure 10. The scientific research areas within the SFA represent long-term programmatic focal points that will generate high quality, science impactful, and Hanford-relevant publications as their primary product. These individual contributions will integrate over the lifetime of the SFA to resolve important, broad-based subsurface science questions and Hanford issues (**Anticipated Accomplishments**). Each research element will be populated with one or more research projects (**Project Abstracts**) managed by a PNNL-ERSD principal investigator (**Biographical Sketches**) with aligned university or national laboratory collaborators (**Collaborator Contributions**) that will have a specific lifetime, depending on the goal. The research projects will align with our science theme (**Concept**), address aspects of our global hypotheses (**Hypotheses**), may focus on one or more Hanford high risk contaminants (U, Tc, Pu; **Key Contaminants and Research Issues**), and will be highly collaborative within and between projects as a fundamental requirement. Individual projects will be initiated, mature and transition through the SFA lifetime depending on accomplishment, review, and SFA needs.

The primary scientific areas include: i.) molecular research on bacterial cells and their reactive macromolecules, mineral nanoparticles and surfaces, and biotic-abiotic interfacial domains; ii.) biotic and mineralogic microenvironments at the sub- and pore scale with emphasis on kinetic reactions, biogeochemical speciation, and coupling with microscopic transport; iii.) laboratory- and meso-scale (through collaboration) reactive transport experiments of microenvironments and transition zones; and iv.) in-situ field experiments. Associated, enabling scientific areas include: i.) microbial ecology; ii.)

reactive transport modeling; and iii.) in-situ structures and reactive transport properties (geophysical characterization). Both primary and enabling activities are of equal scientific merit to the SFA and designed to be interactive and interdependent. The SFA relies strongly on state-of-the-art EMSL experimental and modeling capabilities, and DOE synchrotron measurements of different kind (enabled by three collaborators) for molecular and pore-scale studies. The Hanford IFC provides model system concepts and questions; sediment samples, cores, and blocks for microbiologic and biogeochemical characterization and hydrobiogeochemical laboratory study; and wells and associated infrastructure for in-situ experiments. Additional detail on the primary and enabling scientific areas follow.



Microbial Ecology

An important goal of the PNNL SFA is to develop a conceptual model for microbial ecology in Hanford's unconfined aquifer (underlying the 200 A plateau and in the Columbia River corridor) with specific emphasis on implications to long-term contaminant fate and transport. The first essential element is a characterization (census) of microbial biomass, phylogenetic diversity, and biogeochemically-relevant activities at spatial scales and within transition zones that are meaningful for the SFA. The initial research will emphasize phylogenetic (16S rRNA gene) analysis to: i.) provide rapid identification of Hanford-relevant model systems to inform scientists working on molecular- and pore-scale studies; and ii.) address ecological issues of community richness, equitability, and spatial heterogeneity. Additional quantitative molecular analyses of biogeochemically-relevant functional genes

and analyses of relevant biogeochemical activities will be conducted. EMSL proteomics capabilities will

be applied in later stages to microbial community analyses, most probably from groundwater samples, in order to identify expressed functional capabilities rather than just genomic potential. High-efficiency cultivation-dependent approaches will also be applied with subsurface materials to address ecological questions of organism and community functional redundancy, and to produce isolated microbes or consortia that affect U, Tc, or Pu biogeochemical behavior. These may become subsequent subjects of detailed research in multiple tasks within the SFA from genomic, metabolic and biogeochemical perspectives.

The census activities will be dependent upon opportunities that arise from Hanford drilling campaigns. The first microbial ecology study site will be at the Hanford-Ringold Characterization Borehole that will sample the unconfined aquifer-Columbia River interaction zone (Figure 11) via aseptic collection of a 55 m subsurface core approximately 50 m from the Columbia River. We anticipate that other samples of opportunity (e.g., Pu-contaminated Z-crib sediments) will arise in media of different geological, hydrological and chemical properties through the project period. To the extent that physical and chemical selection forces directly determine phylogenetic and functional richness of microbial communities; certain selection forces will result in organisms that coincidentally affect the fate and transport of U, Tc, and Pu. Targeted analyses of core samples will evaluate spatial heterogeneity of microbial communities (molecular phylogenetics and functionality) at the sub-cm scale, because this heterogeneity determines the distribution of biogeochemical potential.

Experimental work in microbial ecology will relate the findings of laboratory-oriented molecular and pore-scale research within the SFA to field-relevant conditions. Experimental approaches will include the exposure of either natural microbial communities or model metal-reducing isolates (identified from census efforts) to zones that transition between terminal electron acceptors imposed in cm-scale laboratory column experiments. In this way, specific physiological and molecular responses (identified in molecular scale studies) will be validated under conditions that more closely approximate the field. With model organisms for which genomic and/or proteomic information was determined, a high degree

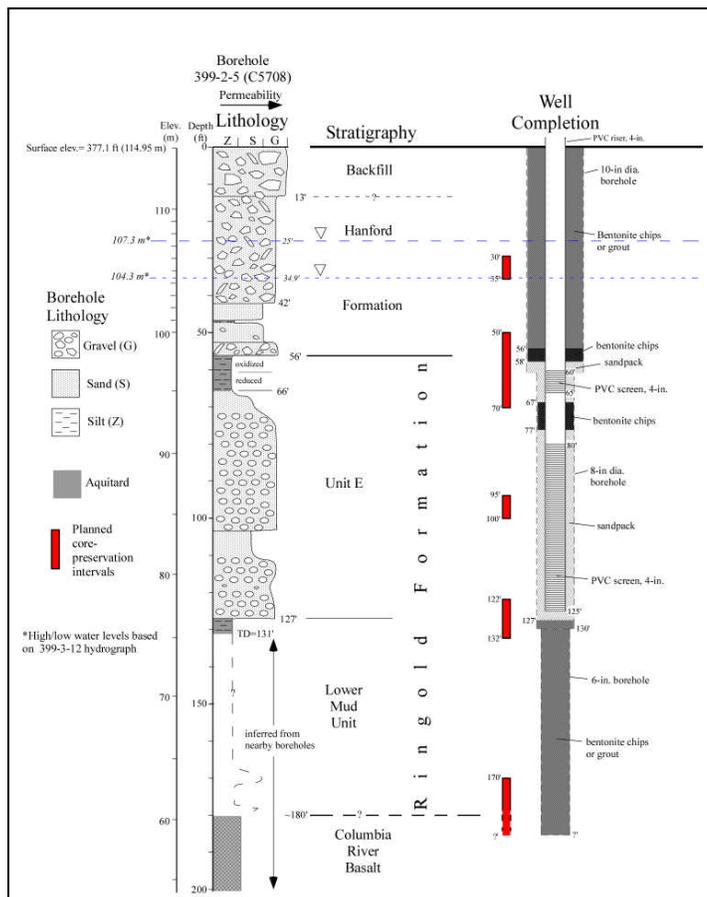


Figure 11. The Hanford-Ringold Characterization Borehole (HRCB) will be installed at the Hanford IFC in 2008, and will sample the noted facies in the Hanford and Ringold Formations. There are a number of dramatic transition zones available for study including the oxic-anoxic zone shown in Figure 4. The HRBC will be a source of samples for microbial ecology and biogeochemical studies. It will be completed as a multi-level monitoring well and represents the first step in the establishment of a transition zone field laboratory that will be developed in collaboration with the Hanford IFC.

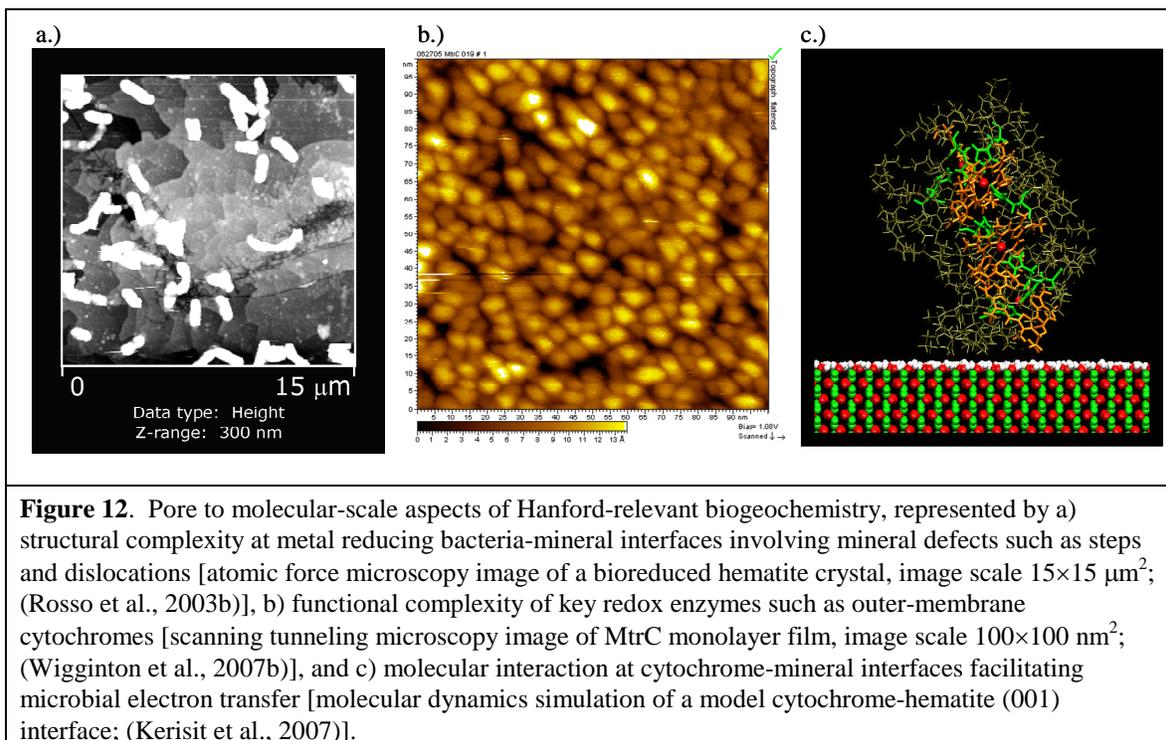
of functional specificity can be addressed via transcriptome and proteome analyses. In experiments with natural communities, molecular analyses of phylogenetic or functional gene markers will be used. The natural evolution of this work will be to proceed to potential field injection experiments and/or to incubations of biological materials (natural communities or metal-reducing isolates) in wells within the Hanford 300 area (see In situ field experiments, below). Similar molecular analyses will be applied as in column experiments, to validate the relevance of molecular-scale mechanisms determined in the laboratory and also to analyze how specific molecular responses determine microbial activity and contaminant mobility under in situ conditions. Technologies that allow specific labeling of microbes that respond to environmental shifts under in situ incubations (for example, stable isotope probing), and which can be analyzed via EMSL analytical capabilities, are especially promising in this regard.

Molecular Scale Studies

Molecular scale research will be performed to advance understanding of the mechanisms and kinetics that underlie the reactivity and transport of U, Tc, and Pu at the Hanford Site. Model systems based on Hanford observations will be used to ensure that fundamental knowledge developed will provide useful environmental insights. Research will focus on key mechanistic research issues at mineral and bacterial interfaces that control biogeochemical behavior of contaminants at the sub-pore, sub-cellular, and microbial cell scale. For example, research will seek basic insights on the molecular: i.) form of the contaminants as soluble species, surface complexes, or discrete phases at key locations at the Hanford Site; ii.) mechanisms of precipitation/dissolution of key contaminant phases (Felmy et al., 2005; Rai et al., 1999), including transformations mediated by abiotic (Kerisit and Rosso, 2006; Kerisit and Rosso, 2007; Rosso et al., 2003a; Rosso et al., 2004; Wander et al., 2006) and microbial electron transfer reactions (Neal et al., 2005; Neal et al., 2003; Rosso et al., 2003b; Smith et al., 2006) [e.g., PuO₂ reduction, U(IV)/Tc(IV) precipitation]; iii.) aspects of reactive Hanford mineral interfaces such as chlorites, magnetite, ilmenite and basaltic glasses containing Fe(II) and Mn(II); and interfaces of U(IV)/Tc(IV) precipitates and PuO₂ (Conradson et al., 2005; Conradson et al., 2004) that control subsequent reactivity and valence cycling; iv.) aspects of intragrain ion diffusion through confined spaces as influenced by charged mineral interfaces; v.) biology of organisms isolated from Hanford subsurface environments with emphasis on those properties and activities impacting contaminant biogeochemistry; vi.) details of microbial cell envelope components and molecular assemblies including catalytic and structural proteins, as well as their distribution and reactive function; vii.) mechanisms that control the biogenesis and extracellular translocation of reactive proteins; and viii.) mechanisms of electron transfer from redox proteins to target contaminants and with Hanford mineral interfaces (Kerisit et al., 2007; Wigginton et al., 2007a; Wigginton et al., 2007b).

A range of bulk and surface spectroscopic and microscopic techniques with high spatial, temporal and/or energetic resolution available in the EMSL and at DOE user facilities will be used to characterize and monitor the molecular structure, chemical composition, and oxidation states of Hanford contaminant species and their mineral or microbial associations through laboratory experiments. Hanford model systems will be used to study surface transformation processes and interfacial reaction products resulting from electron transfer between sorbed or structural Fe(II) with contaminants to examine a range of processes from pure surface passivation [e.g., the reaction product can be soluble: Pu(IV) reduction to Pu(III); (Boukhalfa et al., 2007; Felmy et al., 1989; Rai et al., 2002; Rai et al., 2007), CCl₄ reduction of CHCl₃] to co-precipitation [e.g., formation of mixed Fe(III)-U(IV) or Fe(III)-Tc(IV) coatings; (Peretyazhko et al., 2008; Zachara et al., 2007b)]. Biological methods, including molecular biology and genomics techniques, isolation and purification of biomolecules (e.g., proteins and other macromolecules) and their electrochemical, spectroscopic, and structural characterization, and other approaches applied and developed as part of PNNL's Biogeochemistry Grand Challenge (e.g., Figure 12), will be used to identify the reactive proteins interfacing with Hanford mineral surfaces. Understanding will be sought of their molecular structure, orientation, redox properties and energetics at

interfaces; as well as the nature, thermodynamics, and kinetics of chemical exchange between reactive biomolecules or microorganisms and associated contaminant molecules and/or mineral phases.



Molecular modeling capabilities at the EMSL, such as *ab initio* calculations and molecular dynamics simulations, will be used in support of: i.) experimental molecular scale studies of electron transfer processes and biomolecule interactions (Kerisit et al., 2007), and ii.) microscopic studies of intragrain ion diffusion. The predictions from constructed models will help generate hypotheses and design new experiments. In turn, the experimental data will be used to help build and refine the molecular models. This combined experimental/theory research at the molecular-scale will link with other science areas such as pore scale studies by providing quantitative mechanistic and kinetic insight into Hanford-specific mineral and contaminant transformation reactions, rates of microscopic diffusion processes, and the manners and conditions by which microorganisms promote important biogeochemical processes such as electron transfer and precipitation-dissolution.

Pore Scale Research

Laboratory research will evaluate the linkage of microscopic transport and coupled microbial-geochemical processes involved in the generation of pore-scale microenvironments, micron to millimeter gradients in geochemical and microbiologic properties typically imposed by physical constraints, and reactions of contaminants within them. At the bulk scale, oxic conditions appear to predominate in many Hanford subsurface environments. However, redox conditions at the microscale and across transition zones are, for the most part, unknown. As described in **Background**, reducing conditions are expected in intragrain and other restricted environments where ubiquitous ferrous-containing mineral solids are present, and where oxygen may be consumed by heterogeneous reactions and microbial respiration. Research in this element will span conditions ranging from fully aerobic (i.e., O_2 -saturated) to below the Fe(III)-Fe(II) redox couple, and will include microaerobic conditions believed common to many regions of the unconfined aquifer at Hanford.

Oxidation/reduction and precipitation/dissolution reactions involving the target polyvalent contaminants will be investigated in various types of mineral and biotic Hanford-relevant microenvironments (Figure 13, for example). Investigations will probe the influence of diffusive mass transfer of reactants and products through interconnected pores or grain fractures, as well as within microbial biofilms or microcolonies, on overall reaction kinetics and products.

Understanding the cycling of primary oxidants [O₂,

Mn(III/IV), Fe(III)] and reductants [Fe(II), Mn(II)] within these zones in response to heterogeneous reactions on mineral surfaces and microbiologic activity of different forms, and their coupling to contaminant reactivity will be an emphasis. PNNL has established considerable expertise on these topics through previous ERSP, NABIR, and EMSP supported research including studies addressing Hanford-specific, fundamental science issues. Notable examples include microscale controls on uranium transport, speciation, and reactivity (Fredrickson et al., 2002; Ilton et al., 2008; Liu et al., 2006a; Liu et al., 2004a; Liu et al., 2006b; Liu et al., 2007; Marshall et al., 2006; McKinley et al., 2006); biogeochemical processes controlling technetium solubility (Fredrickson and Zachara, 2008; Fredrickson et al., 2004b; Marshall et al., 2008; Wildung et al., 2004); and heterogeneous electron transfer reactions of Tc (Peretyazhko et al., 2008; Zachara et al., 2007b). PNNL's SFA research will build upon established expertise and scientific knowledge.

New knowledge derived from biogeochemical and microbial ecology investigations at the 300A IFC and other Hanford sites will be used to update pore scale research questions and hypotheses as the SFA evolves. State-of-science analytical capabilities associated with DOE user facilities will be used to define the intricacies of molecular speciation of both contaminants and reactants [e.g., Fe(II/III)] as needed to identify and parameterize fundamental reaction networks, and solute diffusion behavior within intragrain or intracoating pore or fracture spaces and within microbial biofilms or microcolonies. These facilities include EMSL (e.g., microbeam X-ray diffraction, Mössbauer and laser-based spectroscopies, scanning probe and electron microscopies), the Advanced Photon Source (APS) at Argonne National Laboratory (through collaborations), and the Stanford Synchrotron Radiation Laboratory (SSRL) (through collaborations). Broadband geophysical measurements (e.g., electrical impedance, complex resistivity) will be used to characterize spatial and temporal variations in these processes, to understand the relationship between sediment microstructure and hydrogeophysical properties, and for developing accurate upscaling procedures for heterogeneous sediments.

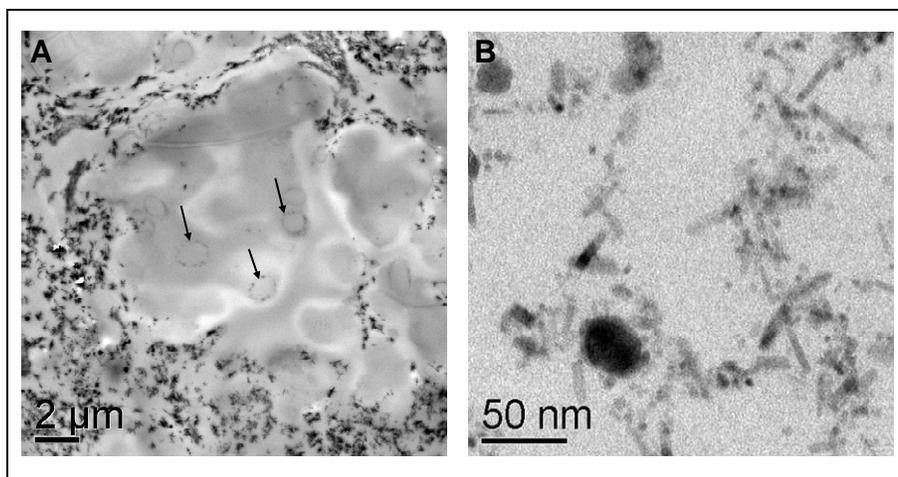


Figure 13. Transmission electron micrographs of thin sections of *Geobacter sulfurreducens* incubated with ferrihydrite and ⁹⁹Tc(VII)O₄⁻. *Geobacter* reduced TcO₄⁻ via a direct enzymatic mechanism to nanoparticulate Tc(IV)O₂, which accumulated within the cell envelope (arrows in A), as well as the ferrihydrite to nanoparticulate Fe(III)/(II) biomineralization products (B). The fine-grained biomineralization products in B contain trace amounts of Tc, as determined by EDS, possibly as a Fe-Tc(IV) phase resulting from biogenic Fe(II)-facilitated reduction of Tc(VII)O₄⁻.

Experimental materials will include representative organisms derived from Hanford subsurface microbial ecology investigations (Figure 14), Hanford subsurface sediments and mineral separates, and model mineral phases and microorganisms. Mineral isolates and aggregates from Hanford exhibiting interconnected pore and grain fracture features of interest will be used, as will constructed pore and fracture networks, to provide well-defined experimental systems with greater experimental control for rigorous hypothesis evaluation and modeling. Laboratory research will be tightly coupled with pore-scale reactive transport modeling to ensure that appropriate data is collected for modeling, and that the models, in turn, provide the framework for information integration, evaluating system understanding, and for transfer to higher scales.

Reactive Transport Experiments

Laboratory research at the macroscopic and meso-scale will seek understanding of the functioning and contributions of microenvironments and transition zones to U, Tc, and Pu migration in sediment-water systems of increasing scale subject to advection (e.g., bulk water movement). The research will utilize centimeter-scale columns of homogeneous porous media; meter-scale flow cells with constructed heterogeneities and transition zones; undisturbed cores collected from the IFC and Hanford waste-site or contaminant plume locations; and excised meter-scale blocks with preserved in-situ features, structures, and heterogeneities. A primary objective will be to explore how diffusion-controlled, microscopic reaction and transport processes couple with advection to regulate contaminant transport in heterogeneous porous media. Experimentation and model formulation will: i.) build strongly on associated and collaborative molecular and pore scale studies performed in other SFA research areas, and ii.) provide important insights on field-scale contaminant transport behavior to be investigated at the IFC and other potential locations. A secondary objective is to investigate the effect of microenvironments and transition zones on geophysical response, and to determine the relation of this response to the determination of effective reactive transport properties and kinetic parameters of different type that can be extrapolated to the field. PNNL and collaborators have a significant track record in this area [e.g., (Ilton et al., 2008; Liu et al., 2008; Pace et al., 2004; Qafoku et al., 2005; Szecsody et al., 1998a; Szecsody et al., 1998b)], and the SFA will build upon, and further refine the sophistication and accomplishments of this research.

Experimentation will seek to characterize zones of mobile and immobile water in Hanford sediments of different properties and configurations, and to specifically identify their respective contributions to contaminant transport in terms of hydrophysical and biogeochemical retardation. The influence of

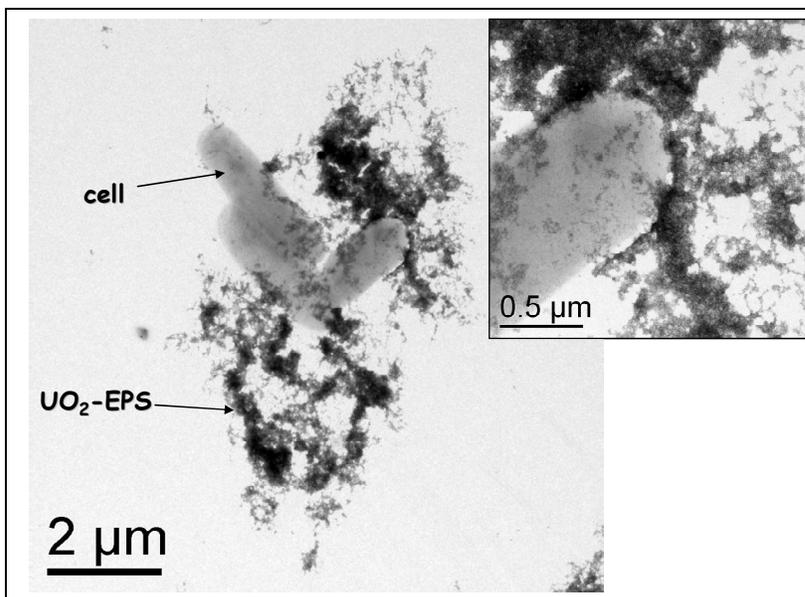


Figure 14. Dissimilatory metal-reducing bacteria have been isolated from Columbia River 300A uranium-seep sediments that have been identified as members of the genus *Shewanella*. These cultures exhibit many of the characteristics of other DMRB including the ability to reduce a wide range of metals and metal oxides. The whole mount TEM images shown here illustrate the end-product of U(VI) reduction by strain HRCR-1, aggregated UO₂ nanoparticles, and their association with extracellular polymer. We anticipate that microbial ecology investigations of Hanford subsurface and hyporheic sediments will yield similar organisms with the capacity for biotransformation of polyvalent metals.

advective water movement and diffusive solute fluxes on the development and function of microsites in coarse textured sediments and transition zones in finer-grained ones will be emphasized within context of field observations made at the IFC with the HRCB. Research will build-upon knowledge gained in molecular and pore scale studies (e.g., molecular mechanisms, geochemical/mineralogic speciation, and biologic/abiotic reaction networks) to interpret reactive transport experiments displaying complex kinetic behavior resulting from the combined effects of mass transfer and biogeochemical reaction. Process coupling is a key consideration, as, for example, the advective supply of reactants and removal of product solutes involved with both abiotic and biotic reaction schemes will strongly influence pore-scale gradients responsible for intragrain/intrapore diffusion, and the directions of involved reactions.

A significant focus will be the characterization of mass transfer processes in terms of fundamental properties controlling apparent diffusivity using: i.) traditional and stop-flow column breakthrough studies of nonreactive and reactive tracers of different molecular diffusivities and charge, and ii.) direct diffusivity measurements of mineral grains using X-ray, NMR, and other spectroscopic techniques. Biogeochemical processes to be studied include precipitation and dissolution in restricted physical domains (both redox and non-redox driven) as commonly observed for U in contaminated Hanford sediments and hypothesized for Tc, and the development of pH and redox zonation at reaction fronts and physical discontinuities. The significant roles of mineral surface chemical reactions (redox and adsorption/nucleation), biologic activity including oxidation of energy sources linked to terminal electron acceptor reduction, and seasonal changes in water chemistry (e.g., nutrients) or temperature will be addressed. The biogeochemistry of both O₂ (heterogeneous and heterotrophic reduction) and Fe(II/III) (heterogeneous reduction and oxidation) will be an important consideration in all experiments as they are closely coupled to the redox states and mobilities of our chosen polyvalent contaminants.

In-Situ Field Experiments

A relatively small but important part of SFA research will be field studies to investigate the in-situ functioning of transition zones, contaminant flux across them in response to advective head gradients and diffusion, and the function of Hanford microbial communities and the environmental factors controlling them. Field research is de-emphasized, but not ignored in the SFA because it is the primary focus of the associated PNNL Hanford IFC.

Both passive (driven by river stage changes) and natural gradient injection experiments will be performed at the IFC in the highly transmissive, U(VI)-contaminated, Hanford formation to evaluate hypotheses related to the dynamics of the in-situ microbial community as influenced by electron donor concentrations (e.g., organic C), nutrient fluxes such as P, and water composition and temperature. This contaminated aquifer unit will be the focus of IFC field experiments targeting multi-scale mass transfer processes influencing in-situ U(VI) adsorption/desorption and transport. Issues of microbial heterogeneity associated with microenvironments will be studied at this highly characterized site where cross-well injection experiments can be performed through subsurface regions of different texture, mineralogy, hydraulic conductivity, and geologic structure (determined nondestructively by geophysical measurement) to assess hydrogeologic influences on in-situ metabolic rates of different type.

Other SFA/IFC field research will target biogeochemical and microbiologic processes, and uranium and other solute fluxes that occur within and across the various types of transition zones that are present at the IFC. These zones include the Hanford formation – Ringold Formation contact, oxic and anoxic zones in the Ringold Formation, and the hyporheic zone where groundwaters and river water actively mix and where seasonal gradients markedly change. The SFA and IFC will jointly install two highly instrumented, multiple-level monitoring well clusters above, within, and below two well defined groundwater transition zones to yield an in-situ, transition zone field laboratory where integrative, multi-investigator field studies can be performed, including a new ERSP research project “Microscale Metabolic, Redox and Abiotic Reactions in Hanford 300 A Subsurface Sediments,” (H. Beyenal, Washington State U., PI). Optimal locations for these well cluster placements and other aspects of

experimental design will be based on results from the HRBC (the major sample source for microbial ecology and biogeochemistry research, e.g., Figure 11) in May-June 2008 and associated microbial ecology research. The well clusters will be instrumented for hourly down-hole monitoring of key analytes, water levels, and temperatures; and used for: i.) passive water quality studies with a diffusion cell string and suspended mineral coupons (described below), or ii.) active tracer experiments using a packing, injection, and pumping configuration to drive cross-zone advection and solute fluxes. Field research concepts, to be closely coupled with microbial ecology/biogeochemistry investigations of IFC sediments from the HRBC, include the use of coupons with different mineralogic coatings to study microbial colonization, potential biomineralization, and subsequent biogeochemical transformations of adsorbed U(VI) and other contaminants.

Future plans call for the establishment of a hyporheic zone laboratory in FY10-11 (in collaboration with DOE/EM) consisting of a dense piezometer network traversing the near-shore aquifer, low water seepage zones, and the near-shore river bed zone to study hydrobiogeochemical processes controlling contaminant and other solute fluxes between groundwater and the Columbia River. Other field locations of opportunity containing either Pu or Tc in the Hanford 200 A plateau will be evaluated for potential field research as the SFA progresses.

Reactive Transport Modeling

Modeling over different spatial scales will be an important and integral component of the SFA. An overall goal of this activity will be the development of a multi-scale modeling approach that incorporates selected abiotic and biotic process models at the sub-pore, pore, and continuum scales. This multi-scale model will closely align with the experimental research tasks that quantify sub-pore and pore scale phenomena associated with microenvironments and transition zones, and their impact on higher scale reactive transport. Modeling will provide: i.) a framework for data and knowledge integration between research elements; ii.) capabilities for experimental simulation as needed for quantification and testing of system understanding in other SFA tasks; iii.) insights on non-linear effects of complex process coupling (e.g., transport, geochemistry, microbiology); and iv.) predictive strength at multiple scales. The model(s) will be a primary tool for interpretation of all experiments in the different research areas.

Ab-initio and molecular dynamics approaches will be used in support of molecular scale studies of electron transfer processes and bio-molecule interactions with mineral surfaces and target contaminants, and microscopic studies of intragrain diffusive processes of different sort. Existing capabilities using grid-based computational fluid dynamics (CFD) and particle-based smoothed particle hydrodynamics (SPH) models (Tartakovsky et al., 2007a; Tartakovsky et al., 2007b; Tartakovsky et al., 2008) will be used to model pore-scale multi-component contaminant reaction and mass transfer processes, and these models will be extended to incorporate key molecular/microscopic phenomena important at this scale as elucidated through experimentation and numerical experiments. In-silico microbial metabolic models will be linked to geochemical reaction and transport models to represent the interplay between microbial function (at individual and community levels) and variations in the local geochemical environment. Continuum biogeochemical reactive transport models such as STOMP will be applied to macroscopic and mesoscopic laboratory transport experiments with quantified heterogeneities, and to field experiments at the Hanford IFC and other locations with their inherent in-situ complexities (Roden and Scheibe, 2005; Scheibe et al., 2006).

Two approaches will be used to incorporate quantitative information and understanding gained from models at smaller scales into these simulations: i.) rigorous upscaling methods (Golfier et al., 2007; Wood, 2007; Wood et al., 2007) will be used to derive continuum-scale models and parameters from small-scale simulation results, and ii.) models at multiple scales will be directly linked within an adaptive hybrid multiscale framework. The latter approach is the focus of PNNL's SciDAC subsurface project, and provides a natural linkage between the SFA and other subsurface computational research funded by ERSP and other DOE entities.

In-Situ Hydrogeologic Structures and Reactive Transport Properties

Research will seek measurement-based, geostatistical methods to extend laboratory-derived knowledge and models of hydrobiogeochemical transport processes (as studied at various scales under idealized conditions in other SFA research areas) to field environments with spatially complex structural features and geologic facies distributions. A long-term objective is to enable characterization of the in-situ reactive transport properties of subsurface zones with complex, sub-meter scale stratigraphy and transition zones (e.g., Figure 5) for implementation and parameterization of multi-scale reactive transport models, as described in the previous section. The general approach is to integrate physical, hydrologic, and geophysical data, with transition probability geostatistics to establish quantitative 3D facies (litho-, hydro-, chemo-, bio-) models of field reactive transport domains (e.g., the 45-m IFC experimental site).

Quantitative spatial information from various borehole, surface, and cross-hole geophysical measurements will be used to map subsurface structural features; while quantitative temporal information obtained through time-lapse measurements of proposed injection experiments will be used to characterize hydrophysical (Kowalsky et al., 2005; Versteeg, 2004; Versteeg and Huang, 2004; Ward et al., 2006) and biogeochemical processes. Surface measurements (electrical resistivity, complex resistivity, ground penetrating radar, self potential, reflection seismic, and terrain conductivity) will be used to delineate transitions between large-scale stratigraphic units (e.g., the Hanford-Ringold contact), as demonstrated by (Sullivan et al., 2007a; Sullivan et al., 2007b), establish general facies patterns, and quantify empirical horizontal transition probabilities (Figure 15). Borehole (thermal neutron, natural gamma spectroscopy, litho-density, array induction), and crosshole (resistivity, radar) measurements will be used to characterize the small-scale facies patterns and vertical transition probabilities (e.g., Figure 11), as necessary to define field-scale microenvironments and transition zones. The application of facies modeling to the description of hierarchical heterogeneity and model parameterization has been demonstrated by team members [e.g. (Murray et al., 2007a; Murray et al., 2007b; Scheibe et al., 2006; Ward et al., 2004)]. Non-invasive, time-lapse imaging using self potential, cross-hole resistivity and radar will be used to map zones of mobile and immobile water and to quantify mass-transfer parameters at multiple scales for independent confirmation of those derived from traditional transport analyses of both laboratory and field experiments.

A key aspect of the research will be the development of correlations between lab- and field-measured geophysical responses and the primary sediment (physical, hydrologic, geochemical, and microbiologic)

properties quantified by ex-situ characterization of whole sediments and their size fractions (e.g., the HRCB; Figure 11). These correlations will be based primarily on laboratory geoelectric measurements (e.g., electrical conductivity) of whole and sieved sediments, and model physical mixtures. These measurements will be used to characterize geometry (porosity, formation factor) and pore-scale lengths important to

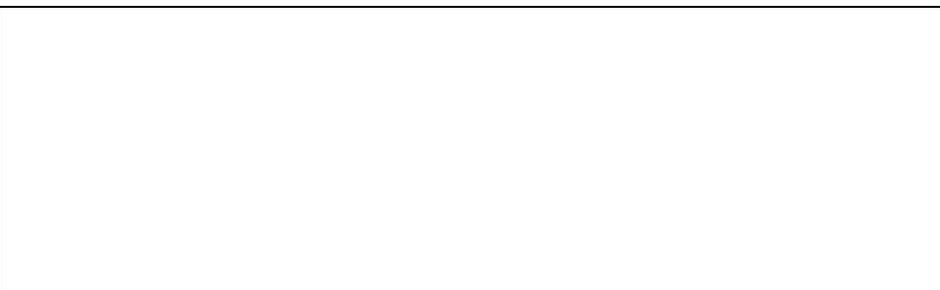


Figure 15. Results of a 2-D surface electrical resistivity survey of a 300 m transect across the 300 A uranium plume near the Hanford IFC. Resistivity response increases from dark blue, to green, to orange, to red. Coarse, dry sediments show high resistivity; while fine textured, water saturated sediments show low resistivity. Backfill exists in the red zone, the water table occurs at yellow, the Hanford-Ringold contact at light blue, and finer-textured Ringold sediments appear as dark blue and black. The geophysical measurements reveal significant subsurface structure (@60-120m and 140-240m) that are interpreted as erosional channels in the Hanford-Ringold contact. Such measurements are essential to define the lateral connectivity and spatial features of transition zones and hydrogeologic structures that control contaminant migration.

transport processes, such as the diffusion-limited surface trapping length and the surface-area-to pore-volume ratio, as functions of water saturation. Measurements will be repeated for each prominent lithofacies to provide independent estimates of reactive transport parameters. This concept builds upon previous EMSP-funded research that demonstrated the use of pore-scale models with particle size information to predict the effective permeability tensor (Stewart et al., 2006); unsaturated hydraulic properties (Tartakovsky et al. 2007); and pore connectivity at the core- (Zhang et al., 2003), and field scales (Ward and Zhang, 2007; Ward et al., 2006; Zhang et al., 2004). The resulting correlations will be used for estimating the geological structures and reactive transport properties of in-situ sediments (e.g., uncured and/or physically inaccessible domains between observation wells) based on surface and/or cross-borehole geophysical measurements. The IFC site and the proposed transition zone field laboratory will be utilized for the development of these diagnostic tools, for the validation of their use in mapping and characterizing subsurface transition zones of different types, and for monitoring of transport processes (Versteeg, 2004; Versteeg and Ankeny, 2004; Versteeg et al., 2000; Versteeg and Huang, 2004). Moreover, derived hydrophysical parameters and inter-well properties and structure estimation (e.g., heterogeneity patterns) will provide key insights necessary for interpretation of field microbial ecology and transition zone experiments. Successful approaches will be subsequently applied to more challenging vadose zone locations in Hanford's 200 A plateau.

Key Contaminants and Associated Research Issues

Approximately 50-60% of the research in the SFA will be directly focused on the subsurface behavior of Hanford contaminants U, Tc, or Pu at different spatial scales. While the SFA organization as portrayed in Figure 11 is based on generic science topics, contaminant specific issues exist that result from the nature of Hanford waste discharges, unique attributes of Hanford's subsurface environment, and the complexity and general state of scientific understanding of the biogeochemistry and reactive transport behavior of each of the target elements. These issues will be a focus of SFA research, and their resolution will assure significant science contribution to the Hanford Site. Selected examples include the following.

Uranium

- Identity and precipitation-dissolution mechanisms/kinetics of U(VI) precipitates formed in Hanford sediments under acidic and basic conditions.
- Coupled adsorption, dissolution, and pore-scale mass transfer processes controlling release kinetics of U(VI) from contaminated sediments
- Surface complexation processes in weathered phyllosilicate aggregates, subsurface sediments with pore infillings of calcium carbonate, and saturated zone sediments containing fractured granitic and basaltic lithic fragments.
- U(VI) biogeochemistry in subsurface microenvironments subject to spatial and temporal variations in redox chemistry as a result of changing lithology, groundwater geochemistry and temperature, and/or microbiologic activities.
- Conditions, responsible organisms, and mechanisms for U(VI) bioreduction in Hanford sediments, and physicochemical and biologic factors controlling reoxidation.
- U distribution between inorganic (mineral) and organic (bacterial) components of hyporheic zone sediments, associated molecular speciation, and seasonal dependencies and fluxes.

Technetium

- Nature of heterogeneous reduction microsites, fundamental electron transfer kinetics from key ferrous-containing mineral phases, and mineral products of Tc(VII) reduction in basaltic and granitic lithic fragments depleted in O₂ through biotic and abiotic reaction.
- In-situ stability of Tc(IV) in aquifer sediment microsites, controlling factors, and evolved phases (such as those containing Fe) that resist oxidation.
- Coupled and competitive biotic and abiotic valence transformations of Tc. Mechanisms of valence species cycling at relevant Hanford redox interfaces.
- Conditions, responsible organisms, and mechanisms for Tc(VII) bioreduction in Hanford sediments.
- Tc distribution between inorganic (mineral) and organic (bacterial) components of hyporheic zone sediments, associated molecular speciation and seasonal dependencies and fluxes.

Plutonium

- Molecular speciation, and physical/mineralogic character, and spatial location of sorbed Pu (adsorbed or precipitated) in Hanford sediments receiving different Pu waste streams.
- Kinetic transformations of Pu [solid phases (surface and bulk); adsorbed phases (species and sorbents); valence (III, IV, V)] associated with long-term, in-ground residence, changing chemical environment resulting from kinetically slow waste-sediment reactions, and long-term, slow microbiologic activity.
- Solubilization and transport mechanisms of Pu in Hanford sediments including abiotic pH extremes, microbiologic activity promoting aqueous complexation or valence change, and colloid formation/migration.
- Biogeochemistry of sediment-sorbed Pu in microsites created by residual saturation with process origin solvents (e.g., carbon tetrachloride and others), or mineralogic products of waste-sediment reaction.

Anticipated Accomplishments

Previous PNNL research leading to the SFA has found that: i.) Hanford contaminants ¹³⁷Cs, U, and ⁹⁰Sr are retained by the sediments in spatially discrete microenvironments resulting from natural processes and waste sediment reaction, and mass transfer controls the rate of their release to the aqueous phase; ii.) active and metabolically-diverse microorganisms exist in Columbia River sediments, the hyporheic zone, and near shore aquifer sediments that are capable of mediating polyvalent metal transformations; and iii.) microenvironments and transition zones at different scales have a controlling effect on water migration. These important results were developed by individual projects where research synergy was not an emphasis. The SFA will perform research differently by aligning a multidisciplinary research team around a broad, but extremely important research theme, and by emphasizing and guiding collaborations around global hypotheses that provide sound scientific structure to the research.

New research will build upon and expand past findings to develop integrating conceptual and numeric models on the role of microenvironments and transition zones in contaminant transport. We will determine primary reaction mechanisms, locations, and transport pathways for Tc and Pu at different scales with the assumption that microenvironments will control their behavior as well. The extremely complex biogeochemistry of U will be further illuminated under different waste chemical regimes, and microscopic information on reaction networks and diffusive transport transferred to field studies at the IFC. The microbial ecology of important subsurface water zones at Hanford will be characterized, and the function of polyvalent metal transforming organisms existing within them studied at various scales under relevant metabolic

conditions to yield new insights on their potential long-term role in contaminant migration and mitigation at Hanford. Hydrobiogeochemical processes within transition zones as shown in Figures 4, and others, will be investigated in different settings, including the field (Figure 11), to understand their role in polyvalent contaminant sequestration and release, and geophysical techniques documented to map their spatial distribution and characterize their reactive transport properties. Multi-scale models will be used to understand complex linkages between chemical, biologic, and physical processes from the molecular to macroscopic scale; to integrate process level understandings and scaling relationships as needed for realistic multi-scale modeling of laboratory and field scale data sets; and to appropriately account for key heterogeneities of different types and dimensions.

These anticipated accomplishments will significantly advance the field of subsurface science, and will support Hanford Site closure by providing knowledge and more robust reactive transport models that will not come from any other source. Indeed, the timing is right for science to impact major, very complex, and controversial cleanup decisions for tank farm closure, U and Tc groundwater remediation, and deep Pu contamination in the vadose zone scheduled in the 2015 time frame.

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Resources and Facilities

The SFA will utilize the following primary locations and capabilities for research. Other important, but unmentioned capabilities reside with our many talented, expert collaborators

Pacific Northwest National Laboratory

The Radiochemistry Laboratory

The radiochemistry laboratories enable batch and flow-cell reactor studies of varying scale using radioactive tracers or contaminated waters and sediments. Dedicated, individual, controlled atmosphere glove boxes exist for U, Tc, and Pu, and approved radiation work protocols exist for the study of these radionuclides. The labs have pH meters, balances, ovens, shakers, centrifuges, wet sieving machines, and controlled atmosphere chambers for studies with desired gas compositions. The radiochemistry laboratory maintains a radiocounting room with state-of-the-art detectors for counting alpha, beta, and gamma emitters. Six high efficiency intrinsic Ge or Ge(Li) detectors are individually housed in special low background steel and lead caves. Other analytical instrumentation is also available including: i.) inductively coupled plasma emission spectrometers (ICP) and ICP-MS (ICP linked to a mass spectrometer) for measuring major cations and trace metals, ion chromatographs and automatic titrators to measure major anions and free hydroxide in solution, multiple X-ray diffractometers for mineral analyses, carbon analyzers, and BET surface area analyzers, and phosphor imaging systems. A dedicated kinetic phosphorescence analyzer (KPA) is available for U(VI) aqueous analyses. A thin section preparation laboratory is maintained for radioactive materials.

The Environmental and Molecular Sciences Laboratory (EMSL/PNNL)

The EMSL is a DOE/BER user facility at PNNL. The facility has advanced capability for environmental molecular sciences as well as: i.) biogeochemistry, mineralogy, and geochemical materials study and ii.) biomolecular characterization. Over 135 different instrumental capabilities are present affording unrivaled opportunities for all disciplines involved in the SFA. These include: an extensive UHV surface science laboratory including various new generation electron microscopies (including SEM, TEM, cryo-TEM, and FIB sample preparation) ideally suited for mineral-microbe studies; a state-of-the-art optical spectroscopy laboratory for environmental materials containing cryogenic stages and optical and confocal microscopes; multiple vibrational spectroscopies and microscopies (FTIR, Raman); various scanning probe microscopies including AFM, STM, and specialized variants; a variable temperature Mossbauer laboratory for iron mineralogy studies with applied field and conversion electron capabilities; numerous molecular and ion-beam spectroscopies for microchemical analyses and imaging mineral surface structure and porosity; and mineral analytical and colloid chemical instrumentation. A mass spectrometry center exists for proteomics and other related analyses of Hanford microorganisms; and a large NMR facility enables protein characterization and other biomolecular studies as well as intragrain diffusion studies with porous media. In addition, computational hardware and software resources are available to perform molecular-based modeling of the interactions between mineral surfaces and microbial cell surfaces, water, and dissolved/solid metal species. This includes all standard *ab initio* and empirical potential modeling techniques (molecular orbital and density functional theory calculations, molecular dynamics simulations), and *ab initio* molecular dynamics, as well as thermodynamic modeling.

EMSL also has a Subsurface Flow and Transport Experimental Laboratory (SFTEL) for porous media physical characterization and automated flow cell or reactive transport experiments at millimeter to meter scales. The facility offers numerous well-engineered and extensively instrumented meter-scale flow cells and columns for research on saturated and unsaturated porous media, a dual-energy gamma

radiation system, and a fully-automated saturation-pressure apparatus. A micro-fluidics laboratory will be developed over the time-period of the SFA.

Environmental Microbiology Laboratories

PNNL maintains a complete suite of capabilities for cultivating aerobic and anaerobic microorganisms and studying the biogeochemical processes they catalyze. These include anaerobic glove bags for cultivating organisms and processing O₂-sensitive sediment cores, anaerobic gassing stations, incubators, and bioreactors of various sizes and configurations. Instrumentation includes: Confocal Laser Scanning Microscopy; epifluorescent microscopy; flow activated cell sorter; kinetic phosphorescence analyzer (for U); liquid scintillation counter; HPLC; GC; FPLC; and reduction gas analyzer. The laboratories are designated for experimental radiological work using various isotopic tracers (e.g., ¹⁴C, ³⁵S, ³H), and radionuclides (U and Tc).

Available facilities for molecular biology techniques include PCR amplification, DNA hybridization analysis, gene cloning, and related techniques. The laboratory has an extensive supply of molecular enzymes and reagents, along with refrigerators and freezers for their storage. Equipment includes four PCR thermocyclers, ABI StepOnePlus for real-time quantitative PCR, an FPLC systems (Amersham Pharmacia Biotech) for protein purification, a denaturing gradient gel electrophoresis system, controlled temperature water baths and incubators, several high-speed centrifuges, and numerous microcentrifuges, an electroporator, and a UV crosslinker for DNA hybridization studies. Electrophoresis equipment, necessary power supplies, fluorescence spectrometers, and digital photograph systems for image capture are available. A microarray core laboratory provides rapid, accurate, and state-of-the-art capabilities. It is equipped with two robotic microarray pin spotters from Apogent (MicroGrid II) and Cartesian Technologies (model PixSys 5500); the ScanArray Express HT imager system (Perkin-Elmer), equipped with 20-slide autoloader and three internal lasers capable of detecting most commercially available fluorescent dyes; an ArrayWorx CCD imager (Applied Precision). In addition an Affymetrix system is available that consists of an Affymetrix® GeneChip® Scanner 3000, Fluidics Station 450, 640 Hybridization Oven, AutoLoader option, and GeneChip® Operating Software (GCOS).

Advanced Photon Source (APS) at Argonne National Laboratory

The SFA will access hard X-ray synchrotron capabilities at APS through ANL collaborators (Kemner and colleagues), and through the beamlines of the former Pacific Northwest Consortia-Collaborative Access Team (PNC-CAT).

The PNC-CAT emphasizes spectroscopic and microbeam measurements in addition to standard diffraction capabilities. A toroidal mirror provides up to 10¹³ ph/sec (5x10¹¹ for the BM line) in a 300 μm spot. Kirkpatrick-Baez mirrors are used to further focus the beam to a spot size of 1-3 μm in diameter containing as many as 10¹² ph/sec. For both cases the focal spot is well separated from the optics allowing for insertion of complex sample environments or cells. X-ray fluorescence is monitored with a 13 element detector. We have successfully performed four major X-ray microprobe (XRM) studies at PNC-CAT looking at the micron-scale spatial distribution of: i.) adsorbed Cs⁺ along the edges and basal surface of Hanford micas and within microfractures in their interstices, ii.) Mn(II), Mn(III), and Mn(IV) in bioreduced Hanford sediments that originally contained todorokite as the primary Mn phase, iii.) Tc(IV) precipitates in Hanford sediments resulting from the redox-reaction of Tc(VI) with sorbed Fe(II) on mineral particles, and iv.) the distribution and identity of micron-sized uranyl silicates within internal grain fractures of granitic lithic fragments isolated from U(VI)-contaminated, deep vadose zone sediment. Log spiral Laue (LSL) detectors have been specifically constructed for U and Tc to allow improved sensitivity. The U-LSL detector has about 90 eV resolution (compared to about 400 eV for the 13 element detector) allowing us to separate U-fluorescence from elements such as Sr that are present in the Hanford sediments at relatively high concentration.

Idaho National Laboratory

INL has a comprehensive suite of geophysical equipment for field measurements in the SFA. These include a 48 channel Geometrics Geode seismic system for seismic refraction mapping, a Geonics EM31, EM38 and EM34 and a Geophex GEM2 for EM induction mapping, a dual channel GPR system from Mala Geoscience with 100, 250, 400 and 800 Mhz antennas for surface GPR mapping and a 180 channel electrical resistivity/IP/SP system from MPT technologies which will be used for the electrical resistivity characterization and monitoring. The GPR system will be able to also run cross borehole GPR antennas, which will be considered for as part of the monitoring options dependent on field tests.

Management and Communications

Organizational Structure of the PNNL Scientific Focus Area (SFA)

The PNNL SFA will include a Technical Research Manager (Dr. Harvey Bolton, Jr.) two chief scientists (Drs. John Zachara (PI) and Jim Fredrickson (Co-PI)), and a core research team. Dr. Bolton in consultation with the Chief Scientists has overall management responsibility of the SFA and interfaces with OBER and PNNL management who have staff in the SFA (Figure 16). Dr. Zachara and Fredrickson will lead and manage the science. The SFA members come from the Fundamental & Computational Sciences Directorate (FCSD), the Energy & Environment Directorate (EED), and the W. R. Wiley Environmental Molecular Sciences Laboratory (EMSL). Dr. Bolton reports directly to Dr. Doug Ray the Associate Laboratory Director of FCSD. Dr. Ray is responsible for all of the programmatic research funding from the DOE Office of Science. Dr. Bolton has been responsible for PNNL research programs funded by the ERSP or its predecessor since 2000.

Capital Equipment

Drs. Bolton, Zachara, and Fredrickson will develop a capital equipment plan for the SFA in consultation with the core research team, OBER, and Dr. Andy Felmy (Chief Scientist from EMSL and member of the SFA) to ensure that capital equipment requests are critical for the SFA and are not duplicative of undersubscribed equipment in EMSL

Management Roles and Responsibilities

Listed below are the key staff in the SFA with their percent commitment and organization in parentheses and science category from Figure 10. A more detailed description of their research role is the Project Abstracts section of the Attachments.

Dr. Harvey Bolton, Jr. (0.25 FTE, FCSD)
Technical Research Manager

Dr. John Zachara (0.47 FTE, FCSD) PI,
reactive transport experiments and in-situ
field experiments

Dr. Jim Fredrickson (0.52 FTE, FCSD) Co-PI,
pore scale

Dr. Don Baer (0.34 FTE, EMSL) molecular
scale

Dr. Alex Beliaev (0.36 FTE, FCSD) molecular
scale and pore scale

Dr. Andy Felmy (0.23 FTE, EMSL) molecular scale

Dr. Alan Konopka (0.20 FTE, FCSD) microbial ecology and in-situ field experiments

Dr. Chongxuan Liu (0.49 FTE, FCSD) pore scale and reactive transport experiments

Dr. Kevin Rosso (0.45 FTE, FCSD) molecular scale

Dr. Tim Scheibe (0.47 FTE, EED) reactive transport modeling

Dr. Liang Shi (0.69 FTE, FCSD) molecular scale

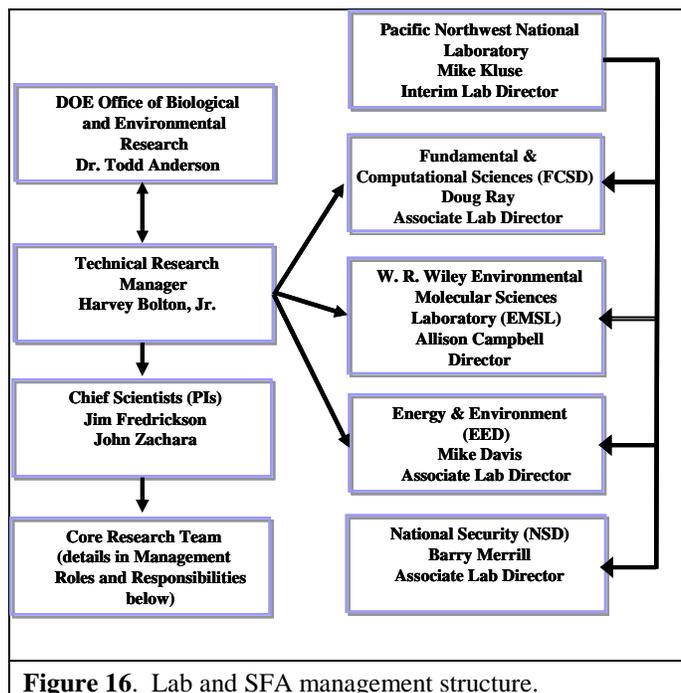


Figure 16. Lab and SFA management structure.

Dr. Andy Ward (0.30 FTE, EED) in-situ structures and reactive transport properties

External Collaborators

Dr. Steve Conradson (LANL), molecular scale

Dr. Jim Davis (USGS), reactive transport experiments and in-situ field experiments

Dr. Scott Fendorf (Stanford University), pore scale and reactive transport experiments

Dr. Ken Kemner (ANL), molecular scale and pore scale

Dr. Rob Knight (University of Colorado), microbial ecology

Dr. Frank Löffler (Georgia Institute of Technology), molecular scale and pore scale

Dr. Melanie Mayes (ORNL), reactive transport experiments and in-situ field experiments

Dr. David Richardson (University of East Anglia), molecular scale

Dr. Eric Roden (University of Wisconsin), pore scale

Dr. Daad Saffarini (University of Wisconsin, Milwaukee), molecular scale and pore scale

Dr. Roloef Versteeg (INL), in-situ structures and reactive transport properties

Dr. Brian Wood (Oregon State University), reactive transport modeling

Communications and Outreach

Internal communications of the SFA will occur primarily through quarterly meetings where research results and management issues will be discussed. An outcome will be a quarterly report to OBER which includes scientific highlights; publications and presentations; an update on goals and milestones for the SFA; anticipated activities during the next quarter; interactions with the public; and any management issues. Edited versions of the reports will be placed on an external SFA web site. This SFA web site will be used to enhance outreach to other institutions and the public and will include components similar to the ERSP funded Hanford Integrated Field Challenge (Hanford-IFC) web site (<http://ifchanford.pnl.gov/>). An annual report summarizing progress and planned activities for the next fiscal year will be discussed with OBER. In addition, Drs. Bolton, Fredrickson, or Zachara will contact OBER to communicate any unusual events or occurrences via telephone and/or email.

Outreach and communication with the rest of PNNL will occur through members of the SFA. Dr. Bolton will communicate the SFA results on a regular basis (e.g., at least quarterly) with line managers of SFA members and other interested managers. Dr. Felmy (Chief Scientist for EMSL) will ensure that open lines of communication exist between the SFA and EMSL. Dr. Terri Stewart is a line manager of staff in the SFA as well as the PNNL manager responsible for interfacing with the EM-22 Groundwater and Soils Remediation Program. Dr. Stewart will be invited to the quarterly internal PI meetings to hear research results and will be copied on all research highlights developed. Additionally, we will participate in joint workshops with the EM-22 Program on metals and radionuclides and modeling as needed. This will ensure that PNNL's Programs funded by OBER and EM-22 are complementary and not duplicative and that science results and site management issues are shared. The Hanford-IFC already attends monthly open meetings conducted by the Hanford Groundwater Remediation Project to communicate progress and new scientific results to Hanford Site remediation contractors, DOE EM staff, regulators, and stakeholders. This SFA will use this existing avenue to communicate significant scientific findings to local officials. Outreach to the scientific community will occur through the web site, publications, presentations and leading symposia at national and international meetings. As an example, Drs. Fredrickson and Konopka are on the organizing committee for the 13th International Symposium on Microbial Ecology to be held in Seattle, Washington in August of 2010.

Budget

DOE F 4620.1 (04-93) All Other Editions Are Obsolete	U.S. Department of Energy Budget Page Fiscal Years 2009-2013	OMB Control No. 1910-1400 OMB Burden Disclosure Statement on Reverse					
ORGANIZATION Pacific Northwest National Laboratory		Budget Page No: 1					
PRINCIPAL INVESTIGATOR (PI)/PROJECT DIRECTOR (PD) Zachara, John M./Fredrickson, James K.		Requested Duration: <u>60</u> (Months)					
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates List each separately with title, A.8 show number in bracket(s)		DOE Funded Person - mps	Funds Requested by Applicant	Funds Granted by DOE			
	<table border="1" style="width: 100%; border-collapse: collapse;"> <tr> <th style="width: 30%;">CAL</th> <th style="width: 30%;">ACAD</th> <th style="width: 30%;">SUMR</th> </tr> </table>	CAL	ACAD	SUMR			
CAL	ACAD	SUMR					
1. Zachara, John M., Sr.Chief Scientist for Environmental Chemistry	26.9		\$ 578,587				
2. Fredrickson, James K, Sr. Chief Scientist for Biological Sciences	27.6		\$ 593,074				
3. Baer, Donald R., Lead Scientist	17.2		\$ 367,365				
4. Bellaev, Alex S.,Sr. Research Scientist	18.8		\$ 239,820				
5. Felmy, Andrew R.Chief Scientist	14.5		\$ 310,713				
6. Konopka, Allan E., Laboratory Fellow	12.1		\$ 261,136				
7. Liu, Chongxuan, Staff Scientist	22.2		\$ 353,865				
8. Rosso, Kevin M, Staff Scientist	21.2		\$ 339,317				
9. Scheibe, Timothy D., Staff Scientist	26.9		\$ 433,908				
10. Shi, Liang, Sr. Research Scientist	39.0		\$ 499,419				
11. Ward, Andy L., Sr. Research Scientist	18.0		\$ 231,183				
12. (32) OTHERS	485.2		\$ 5,233,443				
13. (43) TOTAL SENIOR PERSONNEL (1-8)	729.6		\$ 9,441,830				
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)							
1. (6.5) POST DOCTORAL ASSOCIATES *	358.3		\$ 2,315,666				
2. (1) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)			\$ 84,374				
3. () GRADUATE STUDENTS *			\$ -				
4. () UNDERGRADUATE STUDENTS *			\$ -				
5. (1) SECRETARIAL - CLERICAL			\$ 112,423				
6. (2) OTHER			\$ 154,404				
TOTAL SALARIES AND WAGES (A+B)			\$ 12,108,697				
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)		Included in Above					
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)			\$ 12,108,697				
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM)							
TOTAL PERMANENT EQUIPMENT			\$ 2,443,000				
E. TRAVEL							
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)			\$ 386,663				
2. FOREIGN			\$ 15,165				
TOTAL TRAVEL			\$ 401,828				
F. TRAINEE/PARTICIPANT COSTS							
1. STIPENDS (Itemize levels, types + totals on budget justification page)			\$ -				
2. TUITION & FEES			\$ -				
3. TRAINEE TRAVEL			\$ -				
4. OTHER (fully explain on justification page)			\$ -				
TOTAL PARTICIPANTS () TOTAL COST			\$ -				
G. OTHER DIRECT COSTS							
1. MATERIALS AND SUPPLIES			\$ 1,019,762				
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION			\$ -				
3. CONSULTANT SERVICES			\$ -				
4. COMPUTER (ADP) SERVICES			\$ -				
5. SUBCONTRACTS			\$ 7,157,819				
6. OTHER			\$ 421,410				
TOTAL OTHER DIRECT COSTS			\$ 8,598,991				
H. TOTAL DIRECT COSTS (ATHROUGH G)			\$ 23,552,516				
I. INDIRECT COSTS (SPECIFY RATE AND BASE)		See attachment "Indirect Cost" for explanation.					
TOTAL INDIRECT COSTS			\$ 11,390,484				
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)			\$ 34,943,000				
K. AMOUNT OF ANY REQUIRED COST-SHARING FROM NON-FEDERAL SOURCES			\$ -				
L. TOTAL COST OF PROJECT (J+K)			\$ 34,943,000				

* Section B, lines 1,3, and 4 are third party cost.

U.S. Department of Energy
Budget Page
Fiscal Year 2009

ORGANIZATION Pacific Northwest National Laboratory				Budget Page No: 2	
PRINCIPAL INVESTIGATOR (PI)/PROJECT DIRECTOR (PD) Zachara, John M./Fredrickson, James K.				Requested Duration: <u>12</u> (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates List each separately with title, A-8 show number in bracket(s)				DOE Funded Person - mos	
	CAL	ACAD	SUMR	Funds Requested by Applicant	Funds Granted by DOE
1. Zachara, John M, Sr.Chief Scientist for Environmental Chemistry	5.6			\$ 106,902	
2. Fredrickson, James K, Sr. Chief Scientist for Biological Sciences	6.2			\$ 117,685	
3. Baer, Donald R., Lead Scientist	4.1			\$ 77,448	
4. Bellaev, Alex S.,Sr. Research Scientist	4.3			\$ 48,578	
5. Felmy, Andrew R.Chief Scientist	2.8			\$ 52,636	
6. Konopka, Allan E., Laboratory Fellow	2.4			\$ 46,022	
7. Liu, Chongxuan, Staff Scientist	5.9			\$ 83,920	
8. Rosso, Kevin M, Staff Scientist	5.4			\$ 77,157	
9. Scheibe, Timothy D., Staff Scientist	5.7			\$ 81,353	
10. Shi, Liang, Sr. Research Scientist	8.3			\$ 94,022	
11. Ward, Andy L., Sr. Research Scientist	3.6			\$ 40,743	
12. (32) OTHERS	108.5			\$ 1,051,992	
13. (43) TOTAL SENIOR PERSONNEL (1-8)	162.8			\$ 1,878,458	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (6.5) POST DOCTORAL ASSOCIATES *	77.5			\$ 441,795	
2. (1) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)				\$ 15,888	
3. () GRADUATE STUDENTS *				\$ -	
4. () UNDERGRADUATE STUDENTS *				\$ -	
5. (1) SECRETARIAL - CLERICAL				\$ 21,912	
6. (2) OTHER				\$ 37,568	
TOTAL SALARIES AND WAGES (A+B)				\$ 2,395,621	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				Included in Above	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				\$ 2,395,621	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM)					
TOTAL PERMANENT EQUIPMENT				\$ 365,000	
E. TRAVEL					
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				\$ 81,728	
2. FOREIGN				\$ 2,896	
TOTAL TRAVEL				\$ 84,624	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)				\$ -	
2. TUITION & FEES				\$ -	
3. TRAINEE TRAVEL				\$ -	
4. OTHER (fully explain on justification page)				\$ -	
TOTAL PARTICIPANTS () TOTAL COST				\$ -	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				\$ 228,315	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				\$ -	
3. CONSULTANT SERVICES				\$ -	
4. COMPUTER (ADP) SERVICES				\$ -	
5. SUBCONTRACTS				\$ 1,416,541	
6. OTHER				\$ 86,590	
TOTAL OTHER DIRECT COSTS				\$ 1,731,446	
H. TOTAL DIRECT COSTS (A THRU G)				\$ 4,576,691	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) See attachment "Indirect Cost" for explanation.					
TOTAL INDIRECT COSTS				\$ 2,288,309	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				\$ 6,865,000	
K. AMOUNT OF ANY REQUIRED COST-SHARING FROM NON-FEDERAL SOURCES				\$ -	
L. TOTAL COST OF PROJECT (J+K)				\$ 6,865,000	

* Section B, lines 1,3, and 4 are third party cost.

U.S. Department of Energy
Budget Page
Fiscal Year 2010

ORGANIZATION Pacific Northwest National Laboratory				Budget Page No: 3	
PRINCIPAL INVESTIGATOR (PI)/PROJECT DIRECTOR (PD) Zachara, John M./Fredrickson, James K.				Requested Duration: 12 (Months)	
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates				DOE Funded Person - mos	
List each separately with title, A.8 show number in bracket(s)				Funds Requested by Applicant	
				Funds Granted by DOE	
1. Zachara, John M, Sr.Chief Scientist for Environmental Chemistry				5.2 \$ 107,612	
2. Fredrickson, James K, Sr. Chief Scientist for Biological Sciences				5.4 \$ 110,761	
3. Baer, Donald R., Lead Scientist				3.7 \$ 75,558	
4. Beliaev, Alex S.,Sr. Research Scientist				4.1 \$ 51,162	
5. Felmy, Andrew R.Chief Scientist				3.5 \$ 72,782	
6. Konopka, Allan E., Laboratory Fellow				2.4 \$ 50,086	
7. Liu, Chongxuan, Staff Scientist				4.8 \$ 75,320	
8. Rosso, Kevin M, Staff Scientist				4.6 \$ 71,087	
9. Scheibe, Timothy D., Staff Scientist				5.6 \$ 87,032	
10. Shi, Liang, Sr. Research Scientist				8.3 \$ 102,324	
11. Ward, Andy L., Sr. Research Scientist				3.6 \$ 44,341	
12. (32) OTHERS				94.9 \$ 979,442	
13. (43) TOTAL SENIOR PERSONNEL (1-8)				146.1 \$ 1,827,507	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (6.5) POST DOCTORAL ASSOCIATES *				75.9 \$ 471,215	
2. (1) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)				\$ 15,946	
3. () GRADUATE STUDENTS *				\$ -	
4. () UNDERGRADUATE STUDENTS *				\$ -	
5. (1) SECRETARIAL - CLERICAL				\$ 22,758	
6. (2) OTHER				\$ 32,228	
TOTAL SALARIES AND WAGES (A+B)				\$ 2,369,654	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)				Included in Above	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				\$ 2,369,654	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM)					
TOTAL PERMANENT EQUIPMENT				\$ 578,000	
E. TRAVEL					
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)				\$ 75,837	
2. FOREIGN				\$ 2,964	
TOTAL TRAVEL				\$ 78,801	
F. TRAINEE/PARTICIPANT COSTS					
1. STIPENDS (Itemize levels, types + totals on budget justification page)				\$ -	
2. TUITION & FEES				\$ -	
3. TRAINEE TRAVEL				\$ -	
4. OTHER (fully explain on justification page)				\$ -	
TOTAL PARTICIPANTS () TOTAL COST				\$ -	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				\$ 238,369	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION				\$ -	
3. CONSULTANT SERVICES				\$ -	
4. COMPUTER (ADP) SERVICES				\$ -	
5. SUBCONTRACTS				\$ 1,495,945	
6. OTHER				\$ 81,535	
TOTAL OTHER DIRECT COSTS				\$ 1,815,849	
H. TOTAL DIRECT COSTS (ATHROUGH G)				\$ 4,842,304	
I. INDIRECT COSTS (SPECIFY RATE AND BASE)				See attachment "Indirect Cost" for explanation.	
TOTAL INDIRECT COSTS				\$ 2,235,696	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)				\$ 7,078,000	
K. AMOUNT OF ANY REQUIRED COST-SHARING FROM NON-FEDERAL SOURCES				\$ -	
L. TOTAL COST OF PROJECT (J+K)				\$ 7,078,000	

* Section B, lines 1,3, and 4 are third party cost.

ORGANIZATION Pacific Northwest National Laboratory		Budget Page No: 4	
PRINCIPAL INVESTIGATOR (PI)/PROJECT DIRECTOR (PD) Zachara, John M./Fredrickson, James K.		Requested Duration: <u>12</u> (Months)	
A. SENIOR PERSONNEL: PIPD, Co-PIs, Faculty and Other Senior Associates List each separately with title. A-B show number in bracket(s)		DOE Funded Personnel	Funds Requested
		CAL	by Applicant
		ACAD	by DOE
		SUMR	
1. Zachara, John M., Sr. Chief Scientist for Environmental Chemistry		5.8	\$ 125,371
2. Fredrickson, James K., Sr. Chief Scientist for Biological Sciences		5.4	\$ 116,631
3. Baer, Donald R., Lead Scientist		3.4	\$ 73,987
4. Bellav, Alex S., Sr. Research Scientist		3.8	\$ 49,384
5. Felmy, Andrew R., Chief Scientist		3.1	\$ 67,146
6. Konojka, Allan E., Laboratory Fellow		2.4	\$ 52,740
7. Liu, Chonguan, Staff Scientist		4.3	\$ 69,922
8. Rosso, Kevin M., Staff Scientist		4.1	\$ 67,308
9. Scheibe, Timothy D., Staff Scientist		5.4	\$ 88,251
10. Shi, Liang, Sr. Research Scientist		7.7	\$ 100,565
11. Ward, Andy L., Sr. Research Scientist		3.6	\$ 46,691
12. (B) OTHERS		96.9	\$ 1,053,812
13. (43) TOTAL SENIOR PERSONNEL (1-10)		145.9	\$ 1,911,808
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKET(S))			
1. (6.5) POST DOCTORAL ASSOCIATES *		69.1	\$ 453,312
2. (1) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)			\$ 16,791
3. () GRADUATE STUDENTS *			\$ -
4. () UNDERGRADUATE STUDENTS *			\$ -
5. (1) SECRETARIAL - CLERICAL			\$ 22,655
6. (2) OTHER			\$ 30,140
TOTAL SALARIES AND WAGES (A+B)			\$ 2,434,706
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)		Included in Above	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)			\$ 2,434,706
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM)			
TOTAL PERMANENT EQUIPMENT			\$ 500,000
E. TRAVEL			\$ 76,883
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)			
2. FOREIGN			\$ 3,032
TOTAL TRAVEL			\$ 79,915
F. TRAINEE/PARTICIPANT COSTS			
1. STIPENDS (Itemize levels, types + totals on budget justification page)			\$ -
2. TUITION & FEES			\$ -
3. TRAINEE TRAVEL			\$ -
4. OTHER (fully explain on justification page)			\$ -
TOTAL PARTICIPANTS () TOTAL COST			\$ -
G. OTHER DIRECT COSTS			
1. MATERIALS AND SUPPLIES			\$ 194,345
2. PUBLICATION COSTS/DOCUMENTATION/ISSUANCE			\$ -
3. CONSULTANT SERVICES			\$ -
4. COMPUTER (ADP) SERVICES			\$ -
5. SUBCONTRACTS			\$ 1,415,111
6. OTHER			\$ 80,540
TOTAL OTHER DIRECT COSTS			\$ 1,689,996
H. TOTAL DIRECT COSTS (A THROUGH G)			\$ 4,704,617
I. INDIRECT COSTS (SPECIFY RATE AND BASE) See attachment "Indirect Costs" for explanation.			
TOTAL INDIRECT COSTS			\$ 2,295,383
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)			\$ 7,000,000
K. AMOUNT OF ANY REQUIRED COST SHARING FROM NON-FEDERAL SOURCES			\$ -
L. TOTAL COST OF PROJECT (J+K)			\$ 7,000,000

* Section B, Line #1, 3, and 4 are third party cost.

U.S. Department of Energy
Budget Page
Fiscal Year 2012

ORGANIZATION Pacific Northwest National Laboratory			Budget Page No: 5		
PRINCIPAL INVESTIGATOR (PI)/PROJECT DIRECTOR (PD) Zachara, John M./Frédrickson, James K.			Requested Duration: 12 (Months)		
A. SENIOR PERSONNEL: PIPD, Co-PIs, Faculty and Other Senior Associates List each separately with title, A8s show number in brackets			DOE Funded Person - mos	Funds Requested by Applicant	Funds Granted by DOE
	CAL	ACAD	SUMR		
1. Zachara, John M., Sr Chief Scientist for Environmental Chemistry	5.3			\$ 119,874	
2. Frédrickson, James K. Sr. Chief Scientist for Biological Sciences	5.3			\$ 121,128	
3. Baer, Donald R., Lead Scientist	3.2			\$ 71,768	
4. Beliaev, Alex S., Sr. Research Scientist	3.5			\$ 46,686	
5. Felmy, Andrew R. Chief Scientist	2.7			\$ 62,084	
6. Konojka, Allan E., Laboratory Fellow	2.4			\$ 54,844	
7. Liu, Chongxuan, Staff Scientist	3.8			\$ 65,182	
8. Rosso, Kevin M., Staff Scientist	3.8			\$ 63,911	
9. Scheibe, Timothy D., Staff Scientist	5.1			\$ 87,066	
10. Shi, Liang, Sr. Research Scientist	7.5			\$ 101,776	
11. Ward, Andy L., Sr. Research Scientist	3.6			\$ 48,554	
12. (3) OTHERS	94.2			\$ 1,066,381	
13. (4) TOTAL SENIOR PERSONNEL (1-13)	140.4			\$ 1,909,254	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (6.5) POST DOCTORAL ASSOCIATES *				\$ 466,953	
2. (1) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)				\$ 17,461	
3. () GRADUATE STUDENTS *				\$ -	
4. () UNDERGRADUATE STUDENTS *				\$ -	
5. (1) SECRETARIAL - CLERICAL				\$ 23,559	
6. (2) OTHER				\$ 26,819	
TOTAL SALARIES AND WAGES (A+B)				\$ 2,444,046	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)			Included in Above		
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				\$ 2,444,046	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM)					
TOTAL PERMANENT EQUIPMENT				\$ 500,000	
E. TRAVEL				\$ 78,338	
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN				\$ 3,102	
TOTAL TRAVEL				\$ 81,440	
F. TRAINEE PARTICIPANT COSTS					
1. STIPENDS (itemize levels, types + totals on budget justification page)				\$ -	
2. TUITION & FEES				\$ -	
3. TRAINEE TRAVEL				\$ -	
4. OTHER (fully explain on justification page)				\$ -	
TOTAL PARTICIPANTS () TOTAL COST				\$ -	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				\$ 185,392	
2. PUBLICATION COSTS/DOCUMENTATION/DISEMINATION				\$ -	
3. CONSULTANT SERVICES				\$ -	
4. COMPUTER (ADP) SERVICES				\$ -	
5. SUBCONTRACTS				\$ 1,415,111	
6. OTHER				\$ 84,280	
TOTAL OTHER DIRECT COSTS				\$ 1,684,783	
H. TOTAL DIRECT COSTS (THROUGH G)				\$ 4,710,269	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) See attachment "Indirect Cost" for explanation.					
TOTAL INDIRECT COSTS				\$ 2,289,731	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				\$ 7,000,000	
K. AMOUNT OF ANY REQUIRED COST-SHARING FROM NON-FEDERAL SOURCES				\$ -	
L. TOTAL COST OF PROJECT (J+K)				\$ 7,000,000	

* Section B, lines 1, 3, and 4 are third party cost.

U.S. Department of Energy
Budget Page
Fiscal Year 2013

ORGANIZATION Pacific Northwest National Laboratory			Budget Page No: 6		
PRINCIPAL INVESTIGATOR (PI)/PROJECT DIRECTOR (PD) Zachara, John M./Frédrickson, James K.			Requested Duration: <u>12</u> (Months)		
A. SENIOR PERSONNEL: PIPD, Co-PIs, Faculty and Other Senior Associates List each separately with title, A&S show number in brackets			DOE Funded Personnel	Funds Requested by Applicant	Funds Granted by DOE
	CAL	ACAD	SUMR		
1. Zachara, John M., Sr Chief Scientist for Environmental Chemistry	5.0			\$ 118,827	
2. Frédrickson, James K. Sr. Chief Scientist for Biological Sciences	5.3			\$ 126,869	
3. Baer, Donald R., Lead Scientist	2.9			\$ 68,605	
4. Beliaev, Alex S., Sr. Research Scientist	3.1			\$ 44,009	
5. Felmy, Andrew R. Chief Scientist	2.4			\$ 56,065	
6. Konojka, Allan E., Laboratory Fellow	2.4			\$ 57,444	
7. Liu, Chongxuan, Staff Scientist	3.3			\$ 59,522	
8. Rosso, Kevin M., Staff Scientist	3.4			\$ 59,854	
9. Scheibe, Timothy D., Staff Scientist	5.1			\$ 90,207	
10. Shi, Liang, Sr. Research Scientist	7.1			\$ 100,732	
11. Ward, Andy L., Sr. Research Scientist	3.6			\$ 50,855	
12. (3) OTHERS	90.8			\$ 1,081,815	
13. (4) TOTAL SENIOR PERSONNEL (1-13)	134.4			\$ 1,914,804	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)					
1. (6.5) POST DOCTORAL ASSOCIATES *	67.5			\$ 482,390	
2. (1) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)				\$ 18,289	
3. () GRADUATE STUDENTS *				\$ -	
4. () UNDERGRADUATE STUDENTS *				\$ -	
5. (1) SECRETARIAL - CLERICAL				\$ 21,537	
6. (2) OTHER				\$ 27,649	
TOTAL SALARIES AND WAGES (A+B)				\$ 2,464,669	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)			Included in Above		
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A+B+C)				\$ 2,464,669	
D. PERMANENT EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM)					
TOTAL PERMANENT EQUIPMENT				\$ 500,000	
E. TRAVEL				\$ 73,876	
1. DOMESTIC (INCL. CANADA AND U.S. POSSESSIONS)					
2. FOREIGN				\$ 3,173	
TOTAL TRAVEL				\$ 77,049	
F. TRAINEE PARTICIPANT COSTS					
1. STIPENDS (itemize levels, types + totals on budget justification page)				\$ -	
2. TUITION & FEES				\$ -	
3. TRAINEE TRAVEL				\$ -	
4. OTHER (fully explain on justification page)				\$ -	
TOTAL PARTICIPANTS () TOTAL COST				\$ -	
G. OTHER DIRECT COSTS					
1. MATERIALS AND SUPPLIES				\$ 173,341	
2. PUBLICATION COSTS/DOCUMENTATION/DISEMINATION				\$ -	
3. CONSULTANT SERVICES				\$ -	
4. COMPUTER (ADP) SERVICES				\$ -	
5. SUBCONTRACTS				\$ 1,415,111	
6. OTHER				\$ 88,465	
TOTAL OTHER DIRECT COSTS				\$ 1,676,917	
H. TOTAL DIRECT COSTS (A THROUGH G)				\$ 4,718,635	
I. INDIRECT COSTS (SPECIFY RATE AND BASE) See attachment "Indirect Cost" for explanation.					
TOTAL INDIRECT COSTS				\$ 2,281,365	
J. TOTAL DIRECT AND INDIRECT COSTS (H+I)				\$ 7,000,000	
K. AMOUNT OF ANY REQUIRED COST-SHARING FROM NON-FEDERAL SOURCES				\$ -	
L. TOTAL COST OF PROJECT (J+K)				\$ 7,000,000	

* Section B, lines 1, 3, and 4 are third party cost.

PNNL Budget Explanation

Funding Mechanism

PNNL is to receive all funding identified on the PNNL budget pages.

A./B. Senior Personnel(Support by CV)/Other Personnel (FTE/Year)/Primary Responsibility (FTE commitment given for FY 09 only)

Harvey Bolton, Jr. (0.25 FTE), Technical Research Manager. Dr. Harvey Bolton will serve as the management point of contact between PNNL/SFA and BER/ERSD. He will be responsible for all reporting requirements of the SFA to ERSD. Dr. Bolton will assure that the significant accomplishments of the SFA are relayed to PNNL upper management, and that ERSD guidance and scientific direction is properly relayed to SFA principal investigators.

John M. Zachara (0.47 FTE), Principal Investigator. Dr. John Zachara will serve as Co-Principal Investigator for the SFA with Dr. Jim Fredrickson. The two will jointly manage the science portfolio of the SFA and be responsible for its scientific outcome. Dr. Zachara will coordinate SFA activities with the Hanford site and be responsible for assuring and managing site impact. He will also facilitate all coordination with PNNL's Hanford IFC working toward partnership and synergy on field experiments proposed by both projects. Dr. Zachara is P.I. for the SFA project titled "Reactive Transport of U and Tc in Sediment Systems Containing Microenvironments and Transition Zones". He will participate in research activities related to reactive transport experimentation, biogeochemical transformations of U and Tc, spectroscopic measurements of speciation, and microscopic studies targeting mineralogic residence and association.

Jim K. Fredrickson (0.52 FTE), Principal Investigator. Dr. Fredrickson is the scientific co-lead of the PNNL SFA with Dr. Zachara and has over 20 years experience in subsurface microbiology and environmental biogeochemistry focusing on biological and geochemical controls on metal and radionuclide fate and transport. He will be the scientific lead and coordinator of all external SFA participants. Dr. Fredrickson will also be responsible for the overall technical direction of "Pore-Scale Biogeochemical Processes Controlling Contaminant Fate and Transport" and its interfacing with SFA companion projects and key external collaborators. Dr. Fredrickson will coordinate microbial biomolecular and ecology activities to ensure integration and linkage with contaminant biogeochemistry research. He will also serve as point-of-contact for ERSP researchers desiring Hanford-relevant microbes and sediments for their research.

Donald R. Baer (0.34 FTE), Co-Principal Investigator. Dr. Baer will serve as the principal investigator for the "Impact of the Local Environment and Electron-transfer Initiated Transformations of the Structure and Chemical Properties of Mineral and Contaminant Nanoparticulates" project. Dr. Baer is the Environmental Molecular Sciences Laboratory Lead Scientist for Interfacial Chemistry and has extensive experience in nanoparticle characterization, oxide surface analysis, scanning probe microscopy, and interfacial studies of different type.

Alexander S. Beliaev (0.36 FTE), Co-Principal Investigator. Dr. Beliaev will serve as principal investigator for the SFA project: "Biomolecular Studies of Microbiological Processes Controlling Contaminant Fate and Transport", which includes genetic and physiological characterization of both model and Hanford-specific metal reducing bacteria. He will direct the experimental activities and be responsible for the supervision of a full-time post-doc, interfacing with collaborating SFA projects, data analysis and interpretation, and manuscript writing.

Andrew R. Felmy (0.23 FTE), Co-Principal Investigator. Dr. Felmy will serve as principal investigator for the SFA project: “The Chemical Form and Transformation Reactions of Plutonium in Hanford Soils and Sediments”. He is Chief Scientist for the Environmental Molecular Sciences Laboratory and has long experience in actinide chemistry studies and thermodynamic modeling. He will be responsible for conceptualizing and managing Pu research in a rigorous and safe manner within our 331 Building Radiochemistry Laboratory, interfacing with internal SFA collaborators, and guiding externally performed X-ray absorption spectroscopy studies on Pu-containing Hanford sediments.

Allan E. Konopka (0.20 FTE), Co-Principal Investigator. Dr. Konopka will be principal investigator for the SFA project: “Microbial Ecology”. He will be responsible for design and data interpretation of multiple types of analyses needed to define the potentially complex microbial ecology of Hanford vadose zone and aquifer sediments of different origin. Dr. Konopka will guide associated research on the function of Hanford microorganisms and consortia, and their abilities to mediate transformations of O₂, Mn, Fe, U, Tc, and Pu. He will actively collaborate with other SFA activities investigating the fundamental biogeochemical behavior of Hanford microorganisms.

Chongxuan Liu (0.49 FTE), Co-Principal Investigator. Dr. Liu will be principal investigator for the SFA project: “Microscopic Mass Transfer of U and Tc in Subsurface Sediments”. Dr. Liu has a unique combination of skills involving biogeochemistry, applied mathematics, and coupled reaction transport modeling at different scales. He will direct and coordinate microscopic transport experimental design and measurements, microscopic and spectroscopic characterization of grain and sediment transport properties, microscopic transport modeling, and associated publications. He will be responsible for the development of new microscopic reactive mass transfer models for the Reactive Transport Modeling Project, and coordinating external microscopic reaction and transport studies.

Kevin M. Rosso (0.45 FTE), Co-Principal Investigator. Dr. Rosso will serve as the principal investigator for SFA project: “Molecular Scale Mechanisms of Biogeochemical Electron Transfer Underlying Subsurface U/Tc Valence Transformation and Stability”. He will be responsible for scientific direction and coordination of all abiotic molecular scale studies, and for close collaboration with molecular scale, biochemical research performed by Dr. Shi and external collaborator Dr. Richardson. He will direct the experimental activities of a full-time post-doc to perform surface and chemical characterization of heterogeneous electron transfer systems, and will guide the electron transfer and biomolecular modeling activities of Dr. Kerisit.

Timothy D. Scheibe (0.47 FTE), Co-Principal Investigator. Dr. Scheibe will serve as principal investigator for the SFA project: “Multiscale Reactive Transport Modeling”. In this role, Dr Scheibe will closely coordinate with multiple SFA laboratory projects investigating pore scale reaction and transport processes, and larger scale reactive transport experiments to develop robust coupled process models of porous media systems containing microenvironments and/or transition zones. His research team will provide needed state-of-the-art modeling capabilities for experimental interpretation of these tasks, and in collaboration with Drs. Ward and Wood (OSU), will develop theoretical and measurement-based concepts for upscaling of knowledge and process-based models to the field. Dr Scheibe and his team will apply these robust models to SFA and IFC field experiments.

Liang Shi (0.69 FTE), Co-Principal Investigator. Dr. Shi will serve as principal investigator for the SFA project: “Functional Characterization of Microbial Macromolecules”. As a microbial biochemist, Dr, Shi will develop model macromolecular experimental systems and approaches to study fundamental electron transfer and other bio-directed reaction processes responsible for the biogeochemical transformations of polyvalent metal contaminants by Hanford subsurface microorganisms. He will closely collaborate with other SFA microbiologists (Konopka, Beliaev, and Fredrickson) to identify key, high impact

microorganism and macromolecular systems for research. Dr Shi will purify and characterize the target macromolecules, determine the bio-mechanisms that regulate their distribution and cellular localization, and, in collaboration with the project of Dr Rosso, perform fundamental research on the mechanisms of their interactions with soluble contaminants and various Hanford mineral surfaces.

Andy L. Ward (0.30 FTE), Co-Principal Investigator. Dr. Ward will be the principal investigator for the SFA project: “Facies-based Characterization of Hydrogeologic Structures and Reactive Transport Properties”. Dr. Ward is a soil physicist and geophysicist who deals with properties measurements, geostatistical relationships, and scaling laws for field-scale hydrogeologic and transport models. His project will obtain independent measurements of pore distribution, surface-area-to-pore-volume ratios, and diffusion-limited surface trapping length using geophysical methods (including complex resistivity), establish correlations between geophysical measurements and sediment physical properties, and direct the activities of a full-time post-doc who will integrate all of the data into a general framework for generating 3D, field scale hydrogeologic models of subsurface domains exhibiting complex stratigraphy, microenvironments of different scale, and transition zones.

E. Travel

Funds are requested for Principal and Co-principal Investigators to attend the annual ERSF PI Meeting. Funds are also requested for staff to attend scientific conference to present their results.

F. Trainee/Participant Costs

Not applicable

G. Other Direct Costs

Materials and Supplies: Funds are requested for laboratory supplies and material, including chemicals, electrodes, glassware, and analytical supplies.

Subcontracts: Contracts will be issued to all external collaborators – Steve Conradson, LANL, (\$100K); James Davis, USGS, (\$136.5K*); Scott Fendorf, Stanford University, (\$91K*); Ken Kemner, ANL, (\$150K); Rob Knight, University of Colorado, (\$91K*); Frank Löffler, Georgia Tech., (\$91K*); Melanie Mayes, ORNL, (200K); David Richardson, University of East Anglia, (\$136.5K*); Eric Roden, University of Wisconsin, (\$91K*); Daad Saffarini, University of Wisconsin (\$91K*); Roelof Versteeg, INL, (\$125K); Brian Wood, Oregon State University, (\$113.7K*). See Collaborator Contributions Section. Collaborator funding levels given for FY09. *The total subcontract cost for university collaborators is higher than the noted funding levels because it includes an additional 9.9% PNNL subcontracting fee.

Other: Funds for waste disposal and post-doctoral associate space reimbursement.

I. Indirect Costs

See attached Indirect Cost sheets.

Project Abstracts

The following abstracts, arranged alphabetically by PNNL principal investigator, define initial 3-year research projects for the SFA. Cohesion and linkage between projects is facilitated by the SFA hypotheses and a series of Hanford-relevant contamination scenarios that focus multi-scale investigations on a limited set of documented field problems or issues. Important Hanford-relevant scenarios to be investigated are: i.) redox reactions of O₂, Fe, and Mn with Tc(VII)/Tc(IV), U(VI)/U(IV), or Pu(IV)/Pu(III) in microenvironments with different structure (e.g., fractures versus pores), Fe mineralogy (lithic fragments, mineral grains of different mineralogy and provenance), and microbiologic processes (O₂-consumption and metal reduction/oxidation), ii.) precipitation/dissolution and adsorption/desorption reactions of U(VI) in mass-transfer controlled domains (e.g., grain coatings, fractures, phyllosilicate aggregates, bacterial cell aggregates and extended, porous calcium carbonate precipitates) under water saturated and unsaturated conditions, iii.) microbial ecology (phylogeny, physiology, in-situ activities) and multi-scale biogeochemical reaction (stoichiometry, speciation, kinetics) and transport (diffusion, advection) of Tc and U in transition zones of different types and scales (physical, mineralogic, and redox).

Impact of the Local Environment and Electron-Transfer Initiated Transformations of the Structure and Chemical Properties of Mineral and Contaminant Nanoparticulates (D. Baer, PNNL)

Fundamental information will be obtained on the physical and chemical transformations that occur on and within mineral oxide nanoparticulates due to electron transfer reactions and other interactions with their local environment and how those transformations alter the reactivity of these particles to impact contaminant transport. The nature of the reactive surfaces, the accessibility of reactive sites, and the structures of the surface and interface layers (or whole nanoparticles) often change significantly as particles respond to and react with their local environment (e.g. surface structure alterations, phase changes, passive layer formation). Although environmentally induced changes occur for bulk materials, the nature and rate for the changes can be more dramatic for nano-sized mineral phases. This project will focus on obtaining information about these environmentally mediated transformations and how they alter particle reactivity, electron availability and particle mobility. Natural, model, and biogenic nanoparticles will be used to study of phase transformations, interfacial reaction products and particulate reactivity. The particles to be examined include different sizes of magnetite, iron (hydr)oxide, and biogenic/abiotic nanoparticulate contaminant phases. Electron transfer initiated transformations will be examined using carbon tetrachloride¹, a Hanford Site contaminant, as a probe molecule that reacts to produce soluble reaction products by competing pathways that are believed to be diagnostic of one and two electron transfer reactions. Investigations will rely heavily on surface and nano-scale analysis capabilities available in EMSL including electron microscopy and spectroscopy and reactivity, as well as XAS spectroscopy at the APS and ALS. The team will couple these *ex situ* methods with optical and other *in situ* characterization tools. These studies tie to the projects on electron transfer (Rosso), Pu transformation (Felmy) and pore/molecular scale research (Fredrickson, Beliaev, Shi). This project formally partners with a BES Chemistry Project, "Reaction Specificity of Nanoparticles in Solution" which is seeking a fundamental understanding of the mechanism(s) that control overall reactivity, reaction specificity and fate of iron-based nanoparticles. (¹Reaction studies with carbon tetrachloride are funded by BES.)

Biomolecular Studies of Microbiological Processes Controlling Contaminant Fate and Transport (A. Beliaev, PNNL; D. Saffarini, U of Wisc.; F. Löffler, Georgia Tech.)

Genetic and physiological characterizations will be performed of DOE & Hanford site-relevant subsurface microbial isolates and consortia. Research will focus on single-organism investigations to understand the molecular mechanisms involved in metal and radionuclide biotransformation with the initial emphasis on reduction reactions. An emphasis will be placed on identifying genes, pathways, and subsystems involved in those key reactions, which will ultimately result in developing a comprehensive cross-species model of biological mechanisms. Based on the information and materials derived from the Microbial Ecology project, we will extend our findings to probe key cellular mechanisms involved in contaminant biogeochemical transformations with site-relevant organisms. The ability of indigenous microorganisms to coincidentally catalyze the reduction of key contaminants (U, Tc, and Pu) together with naturally-occurring terminal electron acceptors under conditions relevant to Hanford microenvironments will be investigated to address the SFA research hypotheses. Our integrative approach to studying the molecular mechanisms of metal and radionuclide biotransformation will utilize a combination of genetic, biochemical, and cultivation approaches in conjunction with high-throughput proteomic and genomic technologies. Utilization of EMSL capabilities will also be critical for ultra-high-resolution imaging and localization of redox active proteins on the cell surfaces that promote electron transfer and interactions with mineral phases. In turn, we will provide resources, information, and materials for molecular- and pore-scale studies, including the identity of macromolecules for *in situ* probing of key genes/proteins in environmental samples, their subsequent *in vitro* analyses, and relevant contaminant solids for the nanoparticle project (Baer). Collaborations with Saffarini and Löffler will utilize their expertise in molecular biology and ecology of metal-reducing organisms, respectively, to identify metal-reducing genes in Hanford-relevant organisms. Our research will be closely coordinated with the molecular scale projects (Rosso, Shi) that will isolate and characterize redox active proteins and pore scale projects that will explore biogeochemical processes controlling speciation of U and Tc in sediments and mineral separates from Hanford (Fredrickson, Liu).

The Chemical Form and Transformation Reactions of Plutonium in Hanford Soils and Sediments (A. Felmy, PNNL and S. Conradson, LANL)

Fundamental aspects of Pu (bio)geochemistry will be investigated in contaminated Hanford sediments to provide necessary information on causes and mechanisms of anomalous subsurface migration; and insights on its future in-ground stability, phase or speciation transformations, and solid-liquid distribution in various Hanford subsurface microenvironments. The waste cribs at Hanford received effluent generated from plutonium production activities containing hundreds of kilograms of plutonium which have, in certain instances, migrated deep into the subsurface (60 – 130 feet) with some solutions (discharges to the Z-cribs) high in salts, associated organics (TBP, lard oil) and acidic (pH 2). Access to samples gathered from these sites represents a unique opportunity to evaluate both the chemical form of plutonium in these samples, the aqueous speciation reactions that are likely to occur, and the phase transformations that could occur in neutral to low pH, high salt, potentially reducing microenvironments. Initial studies will focus on microscale characterization of the chemical form and phase distribution of plutonium present in Z-crib samples using XAS spectroscopy (performed by S.D. Conradson, LANL) as well as TEM, SEM and XPS, and digital autoradiography. Laboratory studies will focus on kinetic valence and phase transformations, and speciation reactions of plutonium that may occur under both oxidizing and reducing conditions present in Hanford microenvironments of different scale and type. The laboratory studies will include as many Pu-containing Hanford sediments from different sites as can be

obtained (they are sampled relatively infrequently because of health concern), as well as studies of model materials (e.g., PuO₂, ThO₂) to evaluate project hypotheses on specific speciation, solubility, or electron transfer reactions that influence Pu(IV) reduction or mobilization. These studies couple with research being performed in the molecular tasks related to: the reactivity of magnetite nanoparticles (Baer), surface reactions of polyvalent contaminants on ferrous-containing Hanford mineral solids of different type (Rosso), and microbial census and functional analyses of subsurface microbes at Hanford sites (including contaminated ones, Konopka) for evaluating relevant redox-transforming microbial populations.

Pore-Scale Biogeochemical Processes Controlling Contaminant Fate & Transport (J. Fredrickson, PNNL, K. Kemner, ANL; and E. Roden, U. of Wisc.)

Research will probe Hanford/DOE site-relevant biogeochemical processes controlling the subsurface fate and transport of uranium and technetium, building upon knowledge and expertise derived from previous DOE-sponsored research. Using a combination of laboratory and field investigations, we will explore the hypothesis that subsurface microenvironments will be dominant regions of contaminant reaction by focusing on biogeochemical processes that control chemical speciation and physical state of U and Tc in sediments and mineral separates from Hanford as well as in synthetic mineral phases to provide mechanistic insights. Batch/small reactor experiments will utilize model organisms and relevant microbial isolates and consortia obtained via the Microbial Ecology project and characterized by the Biomolecular Mechanisms project. Chemical, microscopy, and spectroscopy-based methods will probe contaminant speciation at the bulk scale and as well as their interactions with microbial cells, their reactive macromolecules, and sediment particles. Redox processes at the pore scale where physical/chemical heterogeneity and differences in transport of electron donors and acceptors can influence bulk geochemical reactions will be investigated (Roden). X-ray spectroscopy and microscopy capabilities at APS (Kemner) will be used to determine contaminant chemical speciation and distribution in sediments from laboratory experiments and field samples. Initial research focus will be on reduction-oxidation reactions with relevant electron-accepting and donating species to test the hypothesis regarding reductive valence transformations in microenvironments with active microbial populations and reactive mineral phases. Experimental systems will include those that are well-mixed and those that are static to impose diffusional limitations. This project will coordinate field experimentation with the Microbial Ecology and In-situ field projects and will include biogeochemical characterization of selected Hanford subsurface materials. Research will also be closely coordinated with the Liu Pore-Scale project that will focus on mass transfer (diffusion/advection) processes at the pore scale, the Zachara reactive transport project that will probe biogeochemical reactive transport issues in homogeneous & heterogeneous experimental systems, and the Scheibe reactive transport modeling project to ensure that experiments and results interface with developing models.

Microbial Ecology (A. Konopka, PNNL and R. Knight, U of Colorado)

This project will have two primary components: (a) a census of Hanford subsurface microbial communities and (b) experimental manipulations of microbial communities or relevant single organisms under simulated natural conditions or *in situ*. The census will use a suite of culture-independent methods (16S rRNA gene analyses, quantitative PCR of specific functional groups of microbes, and proteomic analyses) to assay the relative abundance of different microbes across natural gradients and transition zones and determine the functional proteins expressed by the organisms. Cultivation techniques that emphasize exposure to low nutrient fluxes typical of subsurface environments will be applied in parallel to obtain and characterize

Hanford-relevant microbes. Key outputs from this project will be relevant cultures and processes for detailed investigation and experiments in other SFA projects. Differences in community composition will be related to geological, geochemical and biogeochemical activity features via new data mining tools (Knight). These will form the basis for hypotheses that drive experimental manipulations in which natural communities or Hanford-relevant organisms are incubated in subsurface sediments either in laboratory columns or deployed in boreholes. We anticipate that spatial and temporal heterogeneities in terminal electron acceptors (TEA) (particularly O₂ and Fe or Mn oxides) will affect the fate and transport of U or Tc. These experiments will interface with molecular-scale studies to determine the extent to which biogeochemically-reactive cell components identified in the laboratory are expressed under natural conditions. The analyses from these experiments will have several prongs: (1) measurement of relevant biogeochemical activities (reduction of natural TEA and radionuclides of interest), (2) quantitative analysis of physiological responses molecules (via transcriptome and/or proteome analyses) for experiments with single species and (3) analysis of community composition shifts for experiments with natural communities. Proteome analyses will use PNNL's AMT tag approach and a "pseudo genomic sequence," a collation from "near neighbor" organisms determined from the 16S rRNA gene census, in the absence of the availability of genome sequence. Bayesian hierarchical networks will be applied to construct probability based community profiles from detected peptide markers. In addition, we will provide input to Reactive Transport Modeling project for incorporating microbial distribution and activity into their models and conduct experiments in simulated natural conditions that can test their model predictions.

Microscopic Mass Transfer of U and Tc in Subsurface Sediments (C. Liu, PNNL and S. Fendorf, Stanford)

Microscopic mass transfer processes and their influence on, and coupling with, geochemical and biogeochemical reactions in subsurface sediments are the target of study. Research will investigate reactive diffusion at pore and sub-pore scales that exerts a fundamental kinetic control on U and Tc reactivity in Hanford sediment microenvironments. Diffusion domains to be considered include intragrain fractures, aggregates, cements, and coating materials with mass flux dominated by abiotic processes; and intra-aggregates and biofilms of microbial agents and minerals with activity/concentration gradients dictated by biological reactions. Molecular dynamic simulations of ions with different size and charge will be performed to determine self-diffusion coefficients in porous media with variable pore sizes and pore surface charges, to provide insights into charge- and species- coupled ion diffusion. Percolation-based analysis will be used to investigate the influence of intragrain pore or fracture connectivity on the apparent diffusion coefficients by integrating molecular self-diffusion coefficients and statistical percolation threshold. Microscopic and spectroscopic measurements of Hanford-sediment diffusion systems will be performed to quantify diffusion properties and validate theoretical calculations. Batch, stirred-flow cell, and short column experiments will be used to evaluate the influence of coupled diffusion and geochemical/biogeochemical reactions in controlling the reactive diffusion rates at the pore-scale (Fendorf). Multi-component, pore-scale reactive diffusion models will be developed to integrate self-diffusion coefficients, charge and species coupling, and pore connectivity effects. The project will actively collaborate with the Fredrickson pore scale and Zachara reactive transport projects, and will target common contamination scenarios to allow information exchange and upscaling. Sub-pore scale reactive diffusion models will be developed for implementation in SFA reactive transport model (Scheibe). Pore-scale simulations performed by the reactive transport modeling project (Scheibe) will support this effort by providing insights on needed scaling approaches to describe reactive diffusion processes in mineralogically complex Hanford sediments. Research will incrementally increase

system complexity in the following order: 1) saturated, microporous environments dominated by abiotic processes, 2) saturated microenvironments with mass flux dictated by biological reactions, and 3) unsaturated microenvironments with mass flux affected by water content and percolation.

Molecular Scale Mechanisms of Biogeochemical Electron Transfer Underlying Subsurface U/Tc Valence Transformation and Stability (*K. Rosso, PNNL; K. Kemner, ANL; and D. Richardson, U of E. Anglia*)

A molecular-scale understanding will be developed of biogeochemical electron transfer reactions affecting the stability of U and Tc in Hanford-relevant microenvironments. The project will focus a combination of laboratory experiments and molecular modeling on select abiotic and microbial electron transfer reactions in coordination with pore-scale and reactive transport biogeochemistry projects (Zachara, Fredrickson, Felmy), the macromolecular characterization project (Shi), the nanoparticle project (Baer), and the diffusive mass transfer project (Liu). We will initially concentrate on three Hanford-relevant U(VI)/Tc(VII) reduction pathways: i.) reduction by abiotic or biogenic Fe(II) sorbed to mineral matter, ii.) direct enzymatic reduction by cytochromes on the outer-membranes of bacteria, and iii.) reduction by structural Fe(II) available in relevant phases such as basalt glass, magnetite, ilmenite, and clinocllore. This project will supply mechanistic insight, quantitative rates and the relative importance of reaction steps, and molecular details of associated end products. Using Hanford-relevant model mineral surfaces, a suite of high-resolution surface analytical and microscopic tools in the EMSL and via collaboration with APS (Kemner) will be used to characterize the chemical speciation, structure, and distribution of reaction products of heterogeneous abiotic reduction of U(VI) and Tc(VII) by sorbed and/or structural Fe(II) with attention to Hanford-relevant system variables such as pH, [Fe(II/III)], and P_{O_2} . In coordination with redox protein function (Shi) and structure determination (Richardson), we will use molecular modeling to develop state-of-the-science simulations of elementary biomolecular electron transfer processes. Molecular modeling will be used as a basis for data interpretation, to test and refine elementary reaction mechanisms, and to assist in the development of kinetic expressions for information transfer to the pore-scale.

Multiscale Reactive Transport Modeling (*T. Scheibe, PNNL, and B. Wood, Oregon State U.*)

Reactive transport simulation models (RTMs) will serve as an integrating element among the experimental elements of the SFA, in particular integrating information from fundamental scales (molecular and pore) to column and field prediction scales. RTMs will provide support for experimental design, be iteratively updated based on new experimental results, and support post-experimental analysis and interpretation. We will initially focus on the Hanford IFC, for which we will develop a field-scale model of U transport that will systematically incorporate information from SFA experiments at smaller scales. Quantitatively linking across these scales is an ambitious goal, but will be enabled by strong coordination of SFA research and ongoing computational advances. U transport behavior at the IFC is believed to be strongly influenced by both microenvironments and transition zones. Our modeling activity will strive to incorporate new process-based knowledge on their function (Fredrickson and Liu) and devise acceptable geostatistical approaches to handle their heterogeneities and scales (Ward). The scale integration process will proceed as follows. We will formulate pore-scale RTMs of the defined Hanford-relevant contaminant scenarios, that incorporate new information from molecular and pore-scale SFA experiments (Rosso, Liu and Fredrickson) and Hanford microbial characterization data (Konopka). We will develop a stochastic model of the nature and spatial heterogeneity of categorical sediment types (hydrofacies) based on SFA

geophysical/geostatistical research (Ward) and other IFC characterization data. For each hydrofacies characteristic particle- and pore-size distributions, pore-scale geometry, and mineralogy will be determined using EMSL and APS facilities (by the SFA collaborative team), and these properties linked with biogeochemical and microscopic process information developed through pore-scale research (Fredrickson and Liu). We will then simulate pore-scale reactive transport using existing modeling capabilities, extended to incorporate relevant processes. Pore-scale model results will be rigorously upscaled using volume averaging (external collaborator Wood) to define continuum-scale models and parameter distributions for each hydrofacies. The upscaled models will be validated using SFA laboratory-scale reactive transport experiments (Zachara), and then used to simulate field-scale reactive transport with an existing continuum code. Predictions will be compared to both SFA and IFC experimental observations to test the models' predictive power and necessary iterations performed. Subsequent modeling focus and development will turn to the biogeochemical behavior of U, Tc, and Pu at other locations and in other sediments (with Felmy, Fredrickson, Liu, and Zachara) that will exhibit different thermodynamic and kinetic behaviors, and associated physical, biologic, and mineralogic controls.

Functional Characterization of Microbial Macromolecules (*L. Shi, PNNL, and D. Richardson, U. E. Anglia*)

Research will investigate the molecular mechanisms by which microbial macromolecules (e.g. proteins and polysaccharides) influence the subsurface transport of U and Tc. This project will initially focus on i) the mechanism(s) of electron transfer (ET) from these macromolecules to the target contaminants and to Hanford-relevant reactive mineral phases, and ii) the mechanism(s) by which these macromolecules are localized to specific cellular or extracellular compartments to contribute to resolution of the hypothesis addressing reductive valence transformations in microenvironments. Selection of macromolecules for detailed investigation will be based on the results from previous investigations and forthcoming results from the Konopka and Beliaev projects. An integrated approach, which includes genomics, genetic, molecular biology and different chromatographic separation methods, will be used to purify the selected macromolecules. The biochemical, biophysical, and structural properties of purified macromolecules, especially their ET properties, will be characterized at PNNL, using EMSL and other capabilities, and by the University of East Anglia (Richardson). The structures of these macromolecules and their inter-molecular interactions in solutions will be analyzed with neutron scattering and reflectivity methods at ORNL (as part of ORNL SFA). The characterization results, such as ET rates from the macromolecules to the contaminants and mineral phases and the effects of environmental conditions on the ET rates, will be used in the development and evaluation of molecular models of ET developed by the Rosso project. In turn, the predictions of the models will help generate new hypotheses and design new characterization experiments. The molecular mechanisms that regulate the biosynthesis, distribution and localization of the selected macromolecules in the microbial cells and microsites will be determined by the combined cellular, proteomic, biochemical and nanobiological methods.

Facies-based Characterization of Hydrogeologic Structures and Reactive Transport Properties (*A. Ward, PNNL, and R. Versteeg, INL*)

Variations in physical, hydraulic, and reactive transport properties are closely linked to the distribution of sedimentary lithofacies and can be discerned from spatial variations in geophysical responses. This project will develop a theoretical framework for the generation of 3D facies models based on the integration of hydrologic, geophysical, and geostatistical data.

The initial focus will be on the development of reliable, physically-based models for predicting medium properties from easily obtained and reliable lithologic input data and high-resolution borehole logs. Whole samples from the IFC, and their component fractions, will be characterized to determine physical, chemical, mineralogical, and electrical properties that will be used to cluster facies according to size and lithology. These data will be used to guide development of pore-scale reactive transport models that will form the basis of the scale integration process (Scheibe). Broadband (.001-1000 Hz) electrical measurements during batch, stirred-flow cell, and short column experiments (with Fredrickson/Liu) will be used to establish relationships between sediment properties (physical, hydrologic, geochemical, microbiologic), transport parameters, and the electrical response. Time-lapse hydrogeophysical measurements during reactive transport experiments (lab and field, Zachara) will be used to independently characterize the pore-scale lengths that govern mass transfer, such as the surface-area-to-pore-volume ratio, self-diffusion coefficients, and the diffusion-limited surface trapping length, as well as geometric indices that control hydraulic properties. Broadband laboratory results will be used to develop correlations between lab- and field-measured geophysical (borehole and surface) responses needed for data interpretation, and to address issues related to the variable resolution of the different geophysical methods. The IFC site will function as a field laboratory for validating the resulting relationships, and associated laws for up-scaling of flow and reactive transport parameters derived from pore-scale modeling and laboratory transport experiments (Scheibe and Zachara). Surface geophysical measurements will be used to map inter-borehole heterogeneity patterns at the transition zone field laboratory and the IFC monitoring array. This data will be collected at different observation scales and will be merged to develop 3D Markov chain models as necessary to interpret planned SFA and IFC field transport experiments. The geophysical, geostatistical, and hydrologic data will be integrated into a general theoretical framework for generating 3D facies models, and for defining the spatial patterns and connectivity's of associated field scale microenvironments and transition zones. Among other uses, the 3-D facies models will be used to conceptualize idealized experimental systems for laboratory studies (Zachara, Fredrickson, Liu), and as a framework for hydrologic and field-scale reactive transport calculations at different scales and over different domains (Scheibe).

Reactive Transport of U and Tc in Sediment Systems Containing Microenvironments and Transition Zones (J. Zachara, PNNL; J. Davis, USGS; and M. Mayes, ORNL)

Larger scale laboratory, and field experiments will be used to investigate how microenvironments and transition zones influence the biogeochemical transport behavior of U and Tc in presence of water advection. Research will link information on contaminant speciation, abiotic and biotic reaction networks of target and co-reactive constituents, and reaction and mass-transfer kinetics, as quantified in pore-scale (Fredrickson) and microscopic transport (Liu) studies of common scenarios, with transport behavior in field-relevant sediment systems. Laboratory column and flow cell experiments ranging from 10 cm to 2 m in size will investigate Hanford-relevant biogeochemical transport scenarios. Experiments will evolve from homogeneous, abiotic sediment studies (in initial research), to more complex structured materials in later years with physical heterogeneities (informed by 3-D facies model(s) of key Hanford subsurface domains, Ward) and active Hanford microorganisms (Konopka and Beliaev). The selected use of undisturbed sediment cores, and excised sediment blocks with preserved in-situ features (Mayes) will provide necessary insights on naturally-structured microenvironments. Transport experiments will involve the migration of controlled-composition and tracer-containing solutions through either uncontaminated or contaminated Hanford sediments of well characterized physical, chemical, microbiologic, and mineralogic properties (also shared by other SFA participants). Resulting contaminant and tracer exchanges [and co-

reactive constituents such as O₂ and Fe(II/III)] with sediment solids will be monitored by in-situ devices along the flow-path, analysis of effluent solutions, and post experiment characterization of solids and microorganisms (if involved). Multi-scale, multi-domain reactive transport modeling (Scheibe) parameterized in part from pore-scale studies (Fredrickson and Liu) will be the primary interpretational tool. Initial Hanford scenarios to be investigated are: i.) heterogeneous O₂ and Tc(VII)/Tc(IV) electron transfer in microenvironments associated with basaltic lithic fragments, both without and with oxygen-consuming microorganisms (with Fredrickson and Beliaev), and ii.) mass-transfer controlled precipitation/dissolution and adsorption/desorption reactions of U(VI) in secondary mineral grain coatings and phyllosilicate aggregates under water saturated and unsaturated conditions (with Liu, and Davis and Mayes). Subsequent laboratory research will investigate the biogeochemical reactivity of U and Tc in transport-controlled, oxic-anoxic transition zones using various IFC cores and model transport systems (with Fredrickson, Konopka, Liu, and Beliaev). The field experimental program will be developed in FY10-11 in collaboration with other SFA participants and the Hanford IFC, beginning with the establishment of the transition zone field laboratory and characterization of its hydrogeologic, geochemical, and microbiologic regime.

Collaborator Contributions

Steve Conradson, LANL

LANL will perform X-ray Absorption Fine Structure (XAFS) spectroscopy measurements to determine the local structure and chemical speciation of the Pu in the laboratory and environmental samples prepared by PNL scientists. Previous XAFS measurements by our group on PuO(2+x) and UO(2+x) have shown that the adventitious O is incorporated as oxo groups concomitant with an increase in the valence and a decrease in the ordering of the actinide ion, in contradiction with calculations and diffraction studies sensitive to the average long range order that locate these O atoms within the cubic holes in the fluorite structure. In both cases these phenomena involve cooperative addition of the O and H₂O in clusters, promoting phase separation, and this nanoscale heterogeneity and the formation of strained interfaces appears to be a critical factor in that biogenically formed nanoparticles too small for this phase separation appear fully ordered. Measurements on PNL samples will test which, if any, of these structural properties are present in the PNL samples.

James Davis, USGS

USGS research will emphasize the study of microenvironments, particularly those associated with intraparticle regions of mineral clasts and the micron- to nanometer-sized pores in particle coatings, carbonate cements, and phyllosilicate aggregates commonly found in Hanford vadose zone and saturated sediments. A primary goal of the work will be the development of appropriate kinetic U reaction models (e.g. surface complexation, dissolution, abiotic redox) to be applied within reactive transport models to describe U fate and transport at the sub-pore, pore, and continuum scales. Experimental approaches will include: 1) kinetic batch reactors with sediment composites, as well as size and mineral separates, as a function of aqueous compositions, 2) flow-thru batch reactors, and 3) reactive transport experiments with flow interruption. Constraints on model parameterization will be based on detailed physical characterizations of sediment samples, including intragranular porosity distributions, differential diffusivities of tracers, and TEM studies of grain coatings and mineral aggregates.

Scott Fendorf, Stanford University

Transporting solutes represent a mass transfer-dependent average of biogeochemical processes that vary on the micron-scale within physically complex structured media of the subsurface. Deciphering both the inherent biogeochemical heterogeneity within sediments along with their impact on contaminant transport requires a multifaceted approach utilizing a host of spectroscopic and imaging techniques in combination with novel experimental systems. To determine (bio)geochemical heterogeneity of native sediments at the aggregate level, we will utilize an integrated interrogation starting with synchrotron-based X-ray tomographic imaging; utilizing a new phase-contrast approach, we will differentiate the chemical states of elements in relation to physical structure. We will then cyro-section the aggregated along chief advective or diffusive flow-lines and utilize micro- X-ray absorption spectroscopy and X-ray diffraction to elucidate the specific phases along transport lines. Further, where appropriate, we can combine the sectioning with fluorescent in-situ hybridization, inclusive of 'quantum dot' labeling, to determine specific bacterial populations in relation to geochemical and physical aspects of the samples.

Ken Kemner, ANL

Hard x-ray absorption fine structure (XAFS) spectroscopy measurements will be made near energies of the U L_{III} and Tc K absorption edges at various beam lines at the Advanced Photon Source to characterize the valence state and local chemical environments of these contaminants. When appropriate, similar measurements at the Fe and Mn K-edges will also be made to characterize the predominant redox-

active constituent elements of the sample. When necessary, hard x-ray microprobes, with spatial resolutions of 0.1 – 1000 microns, will be used to characterize the spatial heterogeneities of elements associated with structures from as small as mineral-microbe interfaces to as large as mm-sized pore structures within samples.

Rob Knight, University of Colorado

Research in the Knight lab focuses on high-throughput tools for sequence analysis, especially microbial community analysis. In particular, we have developed UniFrac, a method for clustering whole microbial communities in terms of the evolutionary distance that separates them, and have successfully used this method to cluster samples from diverse physical environments (including soil) and from the gut microbiomes of humans and other mammals. We have also developed a method of barcoded pyrosequencing, which allows us to split a single pyrosequencing run across hundreds of samples (including advanced error-correction techniques for detecting and correcting errors in sample assignment), and have written software that allows us to take the sequences from a pyrosequencing run directly and perform both phylogenetic- and OTU-based community analysis. We propose to use these tools to understand the variability among the samples in this proposal, and expect to uncover trends both in the overall diversity of the community and in which specific kinds of microbes live in which communities.

Frank Löffler, Georgia Tech.

The studies in Löffler's group will be focused specifically on identification, enumeration, and selected characterization of metal-reducing microorganisms, and organisms with other relevant physiologies in Hanford subsurface and Columbia River hyporheic zone sediments and waters. Isolation and physiological characterization of pure cultures is one of the deliverables which will be conducted in collaboration with the Microbial Ecology project.

Melanie Mayes, ORNL

We will investigate mass exchange of water and contaminants occurring between advective and diffusive flowpaths in field-representative 300 Area Hanford sediments. We will use intact samples to interrogate pore-scale processes involved in contaminant sequestration into and diffusion out of microenvironments which develop within the fine-grained "matrix" embedded between cobbles. Nonreactive tracers with different diffusion coefficients, interfacial area tracers, and U(VI)/Tc(VII) will be applied to the samples under transient, unsaturated conditions in order to determine the role of pore-scale mass transfer upon contaminant mobility in sediments with significant reservoirs of relatively immobile pore regimes.

David Richardson, U. of East Anglia

The University of East Anglia (D. Richardson) proposes a series of multi-disciplinary experiments utilising X-ray crystallography and spectropotentiometry to elucidate the mechanisms of extracellular electron transfer in metal-reducing bacteria. Specifically UEA aims to (i) provide a quantitative description of the macro-molecular interactions within the MtrABC and MtrAB:OmcA complexes in the model metal-reducing bacterium *Shewanella oneidensis* MR-1, (ii) define the redox chemistries of the MtrABC, MtrAB:OmcA and MtrAB complexes and compare them those of the individual proteins, (iii) investigate the role of the conserved, non-heme coordinating cysteine residues in the functional and structural properties of OmcA, MtrC, MtrAB and MtrABC, MtrAB:OmcA, and (iv) complement these thermodynamic descriptions with kinetic measurements of electron transfer across a bilayer/membrane.

Eric Roden, University of Wisconsin

Research at UW will examine microbial communities and biogeochemical phenomena associated with redox cycling of metals and various other organic and inorganic compounds within redox transition zones in subsurface sediments. Of specific interest are the oxidation and reduction of iron and manganese at oxic/anoxic interfaces, as well as in zones where anoxic, nitrate-containing fluids contact aqueous and/or solid-phase reduced iron compounds. Such redox interfacial environments may occur at a variety of scales in situ, including the pore scale where physical/chemical heterogeneity and differences in transport of electron donors and acceptors may influence bulk geochemical conditions (including contaminant fate and transport) in unique and unexpected ways. Experimental reactor systems of varying complexity will be used to test hypothetical reaction paths and to define rate laws relevant to in situ subsurface redox processes at Hanford and other DOE sites. Mineralogical transformations (dissolution, precipitation, etc.) together with standard aqueous/solid-phase wet-chemical determinations will be combined with culture-based and molecular analyses of microbial communities that develop in the reactors. These studies will provide a wealth of experimental data useful for cultivation of ongoing ERSP-funded collaborations with PNNL scientists on reaction-based modeling of coupled physical, chemical, and microbiological processes at various spatial scales in subsurface environments.

Daad Saffarini, University of Wisconsin-Milwaukee

We will use genetic and physiology approaches to identify key genes & proteins as well as related subsystems that may be important for the overall process of metal reduction, including electron transfer, secretion pathways, and cytochrome maturation. Our studies will include both model organisms as well as Hanford-relevant strains that are able to reduce Fe(III), U, and Tc. Mutants deficient in the reduction of these electron acceptors will be isolated, and the disrupted genes will be identified. Surface exposed proteins that are required for metal reduction will be characterized in vivo for their ability to transfer electrons to metals or to attach to the substrate surface.

Roelof Versteeg, INL

INL will utilize laboratory and field geophysical data (including electrical resistivity, induced polarization, ground penetrating radar, self potential, reflection seismic and electromagnetic data) to define structural boundaries and transition zones between facies, and hydrogeologic and in-situ reactive transport properties of Hanford subsurface sediments. Broadband (.001-1000 Hz) electrical measurements will be performed on sediments and cores under static and dynamic conditions. Predictive and interpretative models (both conceptual and numerical) will be applied and/or developed to link the data from the broadband measurements to sediment properties and subsurface processes. INL will participate in the design and performance of geophysical field measurements for 3-D subsurface characterization and plume migration monitoring at the Hanford 300 A and other selected locations. Forward and inverse electrical and electromagnetic geophysical modeling codes will be developed and applied to field and laboratory data for the estimation of subsurface properties and processes which can be utilized for reactive transport modeling. The IFC site will function as a field laboratory and validation site for the initial application of these efforts.

Brian Wood, Oregon State Univ.

Oregon State University (PI: Brian Wood) will develop upscaled (continuum-scale) models and parameters for reactive transport at representative porous media scales and in a variety of structural types. The primary goal of this effort is to link the influence of chemical, physical, and biological heterogeneity at a variety of scales to the observable manifestation of reactive transport in the field. Emphasis will be on (1) the influence of chemical heterogeneity (e.g., reactive microenvironments) on the net rate of biological and/or geochemical reaction in the subsurface, (2) the influence of microscale

transport processes (such as diffusion) on reactive transport, and (3) the role of small-scale mixing on the rates of reaction in subsurface environments . Upscaling will be based on the method of volume averaging, and closure of the upscaled representations will be done numerically. Pore scale numerical models will be done both at OSU, and in collaboration with researchers at PNNL using state-of-the-art computational infrastructure and tools. The primary deliverables of this effort will be (1) development of the theoretical framework for describing particular reactive transport scenarios, (2) guidance for the development of detailed pore-scale simulations for prediction of the upscaled transport and reaction parameters, and (3) publications related to the upscaling efforts (and comparison with data, where available from elsewhere in the SFA, including the Hanford Integrated Field Challenge) in collaboration with researchers at PNNL.

Biographical Sketches

HARVEY BOLTON, JR.

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Pacific Northwest National Laboratories (PNNL)
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EDUCATION

B.S.	1979	Natural Resources	University of Rhode Island
M.S.	1983	Soil Microbiology	Washington State University
Ph.D.	1985	Soil Microbiology	Washington State University

RESEARCH INTERESTS

Dr. Bolton has focused his research career on building multidisciplinary teams that bring chemistry and biology together to address problems in contaminant behavior and elemental cycling in the environment. Dr. Bolton led a multidisciplinary project investigating the molecular biology, enzymology, and microbiology of plutonium-EDTA biodegradation and the influence of EDTA biodegradation on plutonium mobility. Dr. Bolton was also a PI as part of a large DOE multi-Lab Project (PNNL, ORNL, and ANL) focused on enhancing carbon sequestration in terrestrial ecosystems. Dr. Bolton's research involved molecular biologists, microbiologists, soil biochemists, and ecologists at multiple institutions investigating how microbial community structure and function influences C sequestration and N cycling in various ecosystems.

EXPERIENCE

2002 to present	Manager of the Biological Sciences Division consisting of microbiologists, cell biologists, structural biologists, and biochemists. Focus of the Division is on systems biology and technology development for high throughput biology focused on how cells and organisms sense and respond to their environment.
2000 to present	Manager of DOE's Office of Biological and Environmental Research portfolio at PNNL for Environmental Remediation Sciences and Life and Medical Sciences
1997 to 2001	Manager of the Biogeochemistry Department.
1993 to 2001	Technical Group Leader, Environmental Microbiology Group, PNNL.
1990 - 1993	Senior Research Scientist, PNNL.
1987 - 1990	Research Scientist, PNNL.
1985 - 1987	Postdoctoral Research Associate, USDA-ARS, Pullman, WA

MEMBERSHIPS OF PROFESSIONAL SOCIETIES

American Association for the Advancement of Science, American Society for Microbiology, American Chemical Society, Soil Science Society of America, Ecological Society of America

HONOR AND AWARDS

Eagle Scout in Boy Scouts, Alpha Zeta and Phi Beta Phi Honor Societies, Graduated summa cum laude, Lindahl and Landerholm Memorial College of Agriculture Scholarships for graduate students, USDA-ARS Post-Doctoral Fellowship Appointment, Graduate Faculty Appointment at Washington State University

SELECT PEER-REVIEWED PUBLICATIONS

- Smith JL, JM Bell, H Bolton, Jr, and VL Bailey. 2007. The initial rate of C substrate utilization and longer-term soil C storage. *Biology and Fertility of Soils* 44: 315-320
- Zhang, H, J. P. Herman, H. Bolton, Jr., Z. Zhang, S. Clark, and L. Xun. 2007. Evidence that Bacterial ABC-Type Transporter Imports Free EDTA for Metabolism. *Journal of Bacteriology* 189: 7991-7997.
- Bailey VL, JL Smith, and H Bolton, JR. 2006. "Substrate-Induced Respiration and Selective Inhibition as Measures of Microbial Activity in Soils." In *Soil Sampling and Methods of Analysis*. Taylor and Francis, Boca Raton, FL, pp. 515-526.
- Bailey, V.L., J.L. Smith, and H. Bolton, Jr. 2005. 14C Cycling in Lignocellulose-Amended Soils: Predicting Long-Term C Fate from Short-Term Indicators. *Biology and Fertility of Soils* 42:198-206.
- Fansler, S.J., J.L. Smith, H. Bolton, Jr., and V.L. Bailey. 2005. Distribution of two C cycle enzymes in soil aggregates of a prairie chronosequence. *Biology and Fertility of Soils* 42:17-23.
- Bailey, V. L., J. L. Smith, and H. Bolton, Jr. 2003. Novel antibiotics as inhibitors for the selective respiratory inhibition method for measuring fungal:bacterial ratios in soil. *Biology and Fertility of Soils* 38: 154-160.
- Bell, J. M., J. L. Smith, V. L. Bailey and H. Bolton, Jr. 2003. Priming effect and C storage in semi-arid no-till spring crop rotations. *Biology and Fertility of Soils* 37: 237-244.
- Link, S. O., J. L. Smith, J. J. Halvorson, and H. Bolton, Jr. 2003. A reciprocal transplant experiment within a climatic gradient in a semiarid shrub-steppe ecosystem: effects on bunchgrass growth and reproduction, soil carbon, and soil nitrogen. *Global Change Biology* 9:1097-1105.
- Bailey, V.L., A.D. Peacock, J.L. Smith, and H. Bolton, Jr. 2002. Relationships between biomass determined by substrate induced respiration, chloroform fumigation-extraction, and lipid extraction. *Soil Biology and Biochemistry* 34 (9): 1385-1389.
- Bailey, V.L., J.L. Smith, and H. Bolton, Jr. 2002. Fungal to bacterial ratios in soils investigated for enhanced C sequestration. *Soil Biology and Biochemistry* 34 (7): 997-1007.
- Smith, J. L., H. Bolton Jr. and J. J. Halvorson. 2002. Soil properties and microbial activity across a 500 m elevational gradient in a semi-arid environment. *Soil Biology & Biochemistry* 34:1749-1757.
- Bohuslavek, J., J. W. Payne, Y. Liu, H. Bolton, Jr., and L. Xun. 2001. Cloning, sequencing, and characterization of a gene cluster involved in EDTA degradation from the bacterium BNC1. *Applied Environmental Microbiology* 67:688-695.
- Liu, Y., T. M. Louie, J. W. Payne, J. Bohuslavek, H. Bolton, Jr., and L. Xun. 2001. Identification, purification, and characterization of iminodiacetate oxidase from the EDTA-degrading bacterium BNC1. *Applied Environmental Microbiology* 67:696-701.
- Rai, D., H. Bolton, Jr., D. A. Moore, N. J. Hess, and G. R. Choppin. 2001. Thermodynamic model for the solubility of PuO₂(am) in the aqueous Na⁺-H⁺-OH⁻-Cl⁻-H₂O-ethylenediaminetetraacetate system. *Radiochimica Acta* 89:67-74.
- Bolton, Jr., H., L. Xun, and D. C. Girvin. 2000. Biodegradation of synthetic chelating agents. In: D. R. Lovley (Ed) *Environmental Microbe-Metal Interactions*. pp. 363-383. ASM Press, Washington, DC.
- Smith, J. L., and H. Bolton, Jr. 2000. Climate change and carbon pools in a semi-arid ecosystem. In Catania (Ed.) *Energy 2000: The Beginning of a New Millennium*. pp. 1250-1255. Las Vegas, Nevada.
- VanBriesen, J. M., B. E. Rittmann, L. Xun, D. C. Girvin, and H. Bolton, Jr. 2000. The rate-controlling substrate of nitrilotriacetate for biodegradation by *Chelatobacter heintzii*. *Environmental Science & Technology* 34:3346-3353.

JOHN M. ZACHARA

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Chemical & Materials Sciences Division
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EDUCATION

1986 Ph.D., Soil Chemistry, Washington State University
1979 M.S., Soil/Watershed Chemistry, University of Washington
1973 B.S., Chemistry, Bucknell University

EXPERIENCE

Dr. Zachara has performed extensive experimental research on adsorption reactions of organic, metal, and radionuclide contaminants to organic materials, mineral matter, and subsurface materials from different geochemical environments. The research has ranged from fundamental surface chemical and spectroscopic studies in the laboratory to site evaluations of solute mobilization and transport in the field. He has been active in evaluating complex co-contaminant interactions that occur in contaminant mixtures and in applying multi-component adsorption models to contaminant binding in mineralogically complex natural materials. Dr. Zachara's current research is focused on the geochemical behavior of metals and radionuclides, the influence of subsurface microbial processes on mineral surface chemistry and mineralization, and reactive transport chemistry. His research is assisted by applications of electron microscopy, scanning probe microscopy, Mössbauer spectroscopy, laser-induced fluorescence spectroscopy, and x-ray absorption spectroscopy to mineral, microbe, and natural materials study.

PROFESSIONAL AFFILIATIONS

- American Geophysical Union, American Chemical Society, American Association for the Advancement of Science, Clay Minerals Society, Geochemical Society of America

AWARDS AND HONORS

- Elected Fellow of the American Association for the Advancement of Science (AAAS)
- Recipient of US Department of Energy's 2007 Ernest Orlando Lawrence Award in Environmental Science and Technology

RECENT AND ONGOING PROFESSIONAL ACTIVITIES

- Associated Western Universities Distinguished Lecturer, FY 94.
- Chief scientist for DOE's Subsurface Science, Co-Contaminant Chemistry Research (1994 to 1998)
- Past associate editor of the Journal of Contaminant Hydrology
- Member of the Stanford University Synchrotron Radiation Laboratory (SSRL) peer review panel (1994 to present) and Science Advisory Committee (SAC, 2006 to present)
- Member of the NAS/NRC study panel on "Intrinsic Remediation of Groundwater" (1997 to 1999)
- Science and Technology Lead for in-ground contaminants at the Hanford Site (1999 to present)
- Past member of U.S. Department of Energy Office of Biological and Environmental Research (OBER) NABIR Scientific Advisory Panel (1999 to 2003)
- Past associate director of PNNL's Environmental Molecular Sciences Laboratory (1999 to 2003)
- Co-coordinator of PNNL's science grand challenge in biogeochemistry (2003-2007)
- Member of the U.S. Department of Energy, Office of Basic Energy Sciences (OBES) Geosciences Council (beginning in 2008)

PUBLICATIONS (from over 170)

- Fredrickson, J. K., and J. M. Zachara. 2008. Electron transfer at the microbe-mineral interface: A grand challenge in biogeochemistry. *T.J. Beveridge Tribute Issue: Geobiology* (Accepted).
- Ilton, E. S., N.P. Qafoku, C. Liu, D.A. Moore, and J.M. Zachara. 2008. Advective removal of intraparticle uranium from contaminated vadose zone sediments, Hanford, USA. *Environmental Science and Technology* (In press).
- Liu, C., J. M. Zachara, N. Qafoku, and Z. Wang. 2008. Scale-dependent desorption of uranium from contaminated subsurface sediments. *Water Resources Research* (Accepted).
- Peretyazhko, T., J. M. Zachara, B. -H. Jeon, S. M. Heald, and R. K. Kukkadapu. 2008. Heterogeneous reduction of pertechnetate [Tc(VII)] by sorbed Fe(II) on crystalline Fe(III) oxides and layer silicates. *Geochimica et Cosmochimica Acta* (Accepted).
- Zachara, J. M., J. Serne, M. Freshley, F. Mann, F. Anderson, M. Wood, T. Jones, and D. Myers. 2007. Geochemical processes controlling migration of high level wastes in Hanford's vadose zone. *Vadose Zone Journal*, 6(4):985-1003.
- Zachara, J. M., S. M. Heald, B. H. Jeon, R. K. Kukkadapu, C. Liu, J. P. McKinley, A. C. Dohnalkova, and D. A. Moore. 2007. Reduction of pertechnetate [Tc(VII)] by aqueous Fe(II) and the nature of solid phase redox products. *Geochim. Cosmochim. Acta* 71(9):2137-2157.
- Zachara, J. M., J. K. Fredrickson, R. K. Kukkadapu, and Y. A. Gorby. 2007. Anaerobic microbial-mineral processes with Fe(III) oxides: Experimental considerations and approaches. Chapter 4 in *Methods for Investigating Microbial-Mineral Interactions*. CMS Workshop Lectures, Vol. 14, (ed., P. A. Maurice and L. A. Warren), pp. 117-165. The Clay Minerals Society, West Lafayette, IN.
- Arai, Y., M. A. Marcus, N. Tamura, J. A. Davis, and J. M. Zachara. 2007. Spectroscopic evidence for uranium bearing precipitates in vadoze zone sediments at the Hanford 300-Area site. *Environ. Sci. Technol.*, 41(13):4633-4639.
- Bond D. L., Davis J. A., and Zachara J. M. 2007. Uranium(VI) release from contaminated vadose zone sediments: estimation of potential contributions from dissolution and desorption. In *Adsorption of Metals by Geomedia II*(eds. M.O. Barnett and D.B. Kent), pp. 379-420. Academic Press, San Diego.
- Liu, C. L., J. M. Zachara, N. Foster-Mills, and J. Strickland. 2007. Kinetics of reductive dissolution of hematite by bioreduced anthraquinone-2,6-disulfonate. *Environ. Sci. Technol.* DOI: 10.1021/es070768k.
- McKinley, J. P., J. M. Zachara, R. G. McCain, J. Wan, D. E. McCready, and S. M. Heald. 2007. Geochemical controls on contaminant uranium in vadoze Hanford formation sediments at the 200 East Area and 300 Area Hanford. *Vadose Zone J.* 6(4):1004-1017.
- McKinley, J. P., J. M. Zachara, S. C. Smith, and C. Liu. 2007. Cation exchange reactions controlling desorption of $^{90}\text{Sr}^{2+}$ from coarse-grained contaminated sediments at the Hanford formation, Washington. *Geochim. Cosmochim. Acta* 71:305-325.
- Catalano, J. G., J. P. McKinley, J. M. Zachara, S. C. Smith, and G. E. Brown, Jr. 2006. Changes in uranium speciation through a depth sequence of contaminated Hanford sediments. *Environ. Sci. Technol.*, 40(8):2517-2524.
- McKinley, J. P., J. M. Zachara, C. Liu, S. M. Heald, B. I. Prenitzer, and B. W. Kempshall. 2006. Microscale controls on the fate of contaminant uranium in the vadose zone, Hanford Site, Washington. *Geochim. Cosmochim. Acta*, 70(8):1873-1887.

COLLABORATORS

Gordon Brown (Stanford University); Carl Steefel (LBNL); James Davis (USGS); Douglas Kent (USGS); Scott Fendorf (Stanford University); Michael Hochella (Virginia Tech); Yoram Rubin (University of California, Berkeley); Roy Haggerty (Oregon State University); Chunmiao Zheng (University of Alabama); Hailang Dong (University of Miami); Peter Lichtner (LANL); Shelley Kelly (ANL), Susan Brantley (Penn State University), Glenn Waychunas (LBNL).

JAMES K. FREDRICKSON

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EDUCATION

B.S. in Soil Sciences, 1978, University of Wisconsin-Stevens Point; M.S. Soil Sciences, 1992, Washington State University; Ph.D. Soil Microbiology, 1984 Washington State University; Postdoctoral Fellowship, 1985; USDA-ARS, Pullman, Washington.

EXPERIENCE

Dr. Fredrickson specializes in Microbial Ecology and Environmental Microbiology. Since joining Pacific Northwest National Laboratory (PNNL) in 1985, he has focused his research efforts in subsurface microbiology and biogeochemistry. He been responsible for laboratory and field research programs investigating the microbial ecology and biogeochemistry of geologically diverse subsurface environments and is recognized nationally and internationally for these efforts. He currently is a Chief Scientist (Laboratory Fellow – Level VI) within the Biological Sciences Division at PNNL.

While at PNNL, Dr. Fredrickson's research has included the following topics:

- **Microbial Ecology and Biogeochemistry of Subsurface Environments** - Investigations of the structure and function of microbial communities and populations in saturated and unsaturated subsurface environments and their relationship to geochemical, geologic and hydrologic properties. Research has also led to the isolation and characterization of bacterial with novel physiological properties.
- **Microbe-Metal and Microbe-Mineral Interactions** – Investigations of mechanisms of dissimilatory metal reduction emphasizing mechanisms of extracellular electron transfer via outer membrane cytochromes and bioreduction of contaminants and metal oxides.

PROFESSIONAL AFFILIATIONS

- Editor-in-Chief of *Microbial Ecology* (1995-2005).
- Editorial Board Member of *Environmental Microbiology* and *Microbial Biotechnology*.
- Divisional Group III Representative for the American Society for Microbiology (1998-2000).
- Ad hoc reviewer for *Science*, *Geochimica et Cosmochimica Acta*, *Geomicrobiology Journal*, *Journal of Bacteriology*, *Soil Biology and Biochemistry*, *Environmental Science and Technology*, *Canadian Journal of Microbiology*, *Chemical Geology* and *Molecular Ecology*.

AWARDS, HONORS, COMMITTEES

- American Society for Microbiology Foundation Lecturer (1998-2000).
- Elected Member, American Academy of Microbiology (1999).
- Co-chaired a colloquium sponsored by the American Academy of Microbiology, 2004. Systems Microbiology: Beyond Microbial Genomics (report published by the American Academy of Microbiology).
- Chief Scientist for the U.S. Department of Energy's (DOE) Genomics: Genomes to Life program (GTL), since 2005.
- Member of the Committee on the Astrobiology Strategy for the Exploration of Mars (2006-2007).
- Fellow of the American Association for the Advancement of Science since 2007.

PUBLICATIONS (*Recent relevant publications are summarized below*)

- Shi, L., T. C. Squier, J. M. Zachara & J. K. Fredrickson, (2007) Respiration of metal (hydr)oxides by *Shewanella* and *Geobacter*: a key role for multihaem *c*-type cytochromes. *Mol. Microbiol.* **65**: 12-20.
- Lee, J.-H., M.-G. Kim, B. Yoo, N. V. Myung, J. Maeng, T. Lee, A. C. Dohnalkova, J. K. Fredrickson, M. J. Sadowsky & H.-G. Hur, (2007) Biogenic formation of photoactive arsenic-sulfide nanotubes by *Shewanella* sp. strain HN-41. *Proceedings of the National Academy of Sciences*: 0707595104.
- Harthshorne, R. S., B. N. Jepson, T. A. Clarke, S. J. Field, J. Fredrickson, J. M. Zachara, L. Shi, J. N. Butt & D. J. Richardson, (2007) Characterization of *Shewanella oneidensis* MtrC: a cell-surface decaheme cytochrome involved in respiratory electron transport to extracellular electron acceptors. *J. Biol. Inorg. Chem.* **12**: 1083–1094.
- Bretschger, O., A. Obraztsova, C. A. Sturm, I. S. Chang, Y. A. Gorby, S. B. Reed, D. E. Culley, C. L. Reardon, S. Barua, M. F. Romine, J. Zhou, A. S. Beliaev, R. Bouhenni, D. Saffarini, F. Mansfeld, B.-H. Kim, J. K. Fredrickson & K. H. Nealson, (2007) Current Production and Metal Oxide Reduction by *Shewanella oneidensis* MR-1 Wild Type and Mutants. *Appl. Environ. Microbiol.* **73**: 7003-7012.
- Xiong, Y., L. Shi, B. Chen, M. U. Mayer, B. H. Lower, Y. Londer, S. Bose, M. F. Hochella, J. K. Fredrickson & T. C. Squier, (2006) High-Affinity Binding and Direct Electron Transfer to Solid Metals by the *Shewanella oneidensis* MR-1 Outer Membrane *c*-type Cytochrome OmcA. *J. Am. Chem. Soc.* **128**: 13978-13979.
- Shi, L., B. W. Chen, Z. M. Wang, D. A. Elias, M. U. Mayer, Y. A. Gorby, S. Ni, B. H. Lower, D. W. Kennedy, D. S. Wunschel, H. M. Mottaz, M. J. Marshall, E. A. Hill, A. S. Beliaev, J. M. Zachara, J. K. Fredrickson & T. C. Squier, (2006) Isolation of a high-affinity functional protein complex between OmcA and MtrC: Two outer membrane decaheme *c*-type cytochromes of *Shewanella oneidensis* MR-1. *J. Bacteriol.* **188**: 4705-4714.
- Roh, Y., H. Gao, H. Vali, D. W. Kennedy, Z. K. Yang, W. Gao, A. C. Dohnalkova, R. D. Stapleton, J.-W. Moon, T. J. Phelps, J. K. Fredrickson & J. Zhou, (2006) Metal Reduction and Iron Biomineralization by a Psychrotolerant Fe(III)-Reducing Bacterium, *Shewanella* sp. Strain PV-4. *Appl. Environ. Microbiol.* **72**: 3236-3244.
- Marshall, M. J., A. S. Beliaev, A. C. Dohnalkova, D. W. Kennedy, D. A. Saffarini, K. M. Kemner, M. I. Boyanov, B. Lai, D. E. Culley, S. B. Reed, L. Shi, Z. Wang, J. S. McLean, V. Bailey, C. J. Simonson, M. F. Romine, J. M. Zachara & J. K. Fredrickson, (2006) *c*-Type Cytochrome-Dependent Formation of U(IV) Nanoparticles by *Shewanella oneidensis*. *PLoS Biology* **4**: 1324-1333.
- Liu, C., B. Jeon, J. M. Zachara, Z. Wang, A. Dohnalkova & J. K. Fredrickson, (2006) Kinetics of Microbial Reduction of Solid Phase U(VI). *Environ Sci Technol* **40**: 6290-6296.
- Kukkadapu, R. K., J. M. Zachara, J. K. Fredrickson, J. P. McKinley, D. W. Kennedy, S. C. Smith & H. L. Dong, (2006) Reductive biotransformation of Fe in shale-limestone saprolite containing Fe(III) oxides and Fe(II)/Fe(III) phyllosilicates. *Geochim. Cosmochim. Acta* **70**: 3662-3676.
- Fredrickson, J. K. & D. L. Balkwill, (2006) Geomicrobial processes and biodiversity in the deep terrestrial subsurface. *Geomicrobiol. J.* **23**: 345-356.
- Marshall, M. J., A. E. Plymale, D. W. Kennedy, Z. Wang, S. B. Reed, A. C. Dohnalkova, C. J. Simonson, C. Liu, D. A. Saffarini, M. F. Romine, J. M. Zachara, A. S. Beliaev, and J. K. Fredrickson. 2007. Hydrogenase- and outer membrane *c*-type cytochrome-facilitated reduction of technetium(VII) by *Shewanella oneidensis* MR-1. *Environ. Microbiol.* DOI: 10.1111/j.1462-2920.01438.x.

COLLABORATORS

- Investigation of mechanisms of ionizing radiation damage and resistance in bacteria related to intracellular concentrations of Fe and Mn (Dr. M. Daly, Uniformed Services University of the Health Sciences).
- Characterization of microbial cell components involved in the extracellular transfer of electrons during respiration to metals (Dr. David Richardson, University of East Anglia, Norwich, UK).
- Isolation and characterization of novel metal-reducing bacteria (Dr. Tom Kieft, New Mexico Tech; Dr. Jizhong Zhou, University of Oklahoma; Dr. David Balkwill, Florida State University).

DONALD R. BAER

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EDUCATION

University of Illinois, Postdoctoral Fellow, 1974-1976, Department of Physics and Materials Research Laboratory
Cornell University, Ph. D. 1974 Experimental Solid State Physics
Carnegie Mellon University, BS, 1969, Physics

EXPERIENCE

Since joining PNNL in 1976, Dr. Baer has specialized in the use of surface sensitive techniques to study how the interactions of a material with its environment alter material properties. Much of his research has involved understanding the roles of surface impurities or contaminants on the chemical reactivity and mechanical properties of minerals and other materials. Specific research activities of Dr. Baer include study of the reaction properties and environmental variability of nanoparticles, synthesis and properties of oxide nanostructures, corrosion and stress corrosion cracking, and the surface chemistry and reactivity of calcite. He has direct experience with vacuum-based surface analysis methods (XPS, AES, UPS, and low energy electron diffraction) and methods used for direct analysis of the solid-solution interface (atomic force microscopy, electrochemical characterization). His research also involves the use of electron microscopy and x-ray adsorption spectroscopy.

PROFESSIONAL AFFILIATIONS

- American Chemical Society
- American Physical Society
- American Vacuum Society (Fellow and Past Chair of the Applied Surface Science Division)
- Geochemical Society of America
- The Electrochemical Society

RELEVANT PROFESSIONAL ACTIVITIES

- Adjunct Professor of Chemistry, University of Washington
- Adjunct Professor of Physics, Washington State University
- Co-Director, University of Washington and PNNL Joint Institute for Nanoscience (2001-2006)
- Deputy Director, PNNL Initiative on Nanotechnology (2001-2006)
- Project Manager of the team responsible for developing materials and interface capabilities for the EMSL (1989-1997)
- Guest Editor Special Issue "The Science and Spectroscopy of Environmentally Important Interfaces" of the *Journal of Electron Spectroscopy and Related Phenomena* 150(2-3) 2006.
- Associate Editor for *Surface Science Spectra* (from 1991), Editorial Board of *Surface and Interface Analysis* (from 2006), Associate Editor, *Journal of Vacuum Science and Technology A*, 1989-1992
- Chair, ASTM Committee E42 on Surface Analysis (2004 ---)
- Coordinator of intensive courses on nanoscience and nanotechnology in collaboration with the University of Washington and Washington State University including the "Synthesis and characterization of nanostructured materials"
- Advisory Board US-Korea NanoForum (2004----)
- International Advisory Board for Practical Surface Analysis 2007, Kanazawa Japan

SELECTED PUBLICATIONS (from over 200):

- Sarathy, V., P. G. Tratnyek, J. T. Nurmi, D. R. Baer, J. E. Amonette, C-M. Wang, C. Chun, R. L. Penn, G. Lai, and E. J. Reardon, 2008, Aging of Iron Nanoparticles in Aqueous Solution: Effects on Structure and Reactivity, *Journal of Physical Chemistry C* in press.
- Baer, D. R., J. E. Amonette, M. H. Engelhard, D. J. Gaspar, A.S.Karakoti, S. Kuchibhatla, P. Nachimuthu, J. T. Nurmi, V. Sarathy, S. Seal, P. G. Tratnyek, and C-M Wang, 2007, Characterization Challenges for Nanomaterials, *Surface and Interface Analysis* in press.
- Wang, C-M., D.R. Baer, J.E. Amonette, M.H. Engelhard, Y. Qiang, and J. Antony, 2007. "Morphology and Oxide Shell Structure of Iron Nanoparticles Grown by Sputter-Gas-Aggregation" *Nanotechnology* 18 (2007) 255603 (7pp)(designated by journal as paper of special interest and journal cover).
- Wang C-M., D.R. Baer, J.E. Amonette, M.H. Engelhard, J. Antony, and Y. Qiang. 2007. "Electron Beam Induced Thickening of the Protective Oxide Layer around Fe Nanoparticles." *Ultramicroscopy* 108, 43–51.
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- Wang C-M., D.R. Baer, L.E. Thomas, J.E. Amonette, J. Anthony, Y. Qiang, and G. Duscher. 2005. "Observation of Void Formation during Early Stages of Passivation: Initial Oxidation of Iron Nanoparticles at Room Temperature." *Journal of Applied Physics* 98, 094308
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- McGrail B.P., J.P. Icenhower, D.K. Shuh, P. Liu, J.G. Darab, D.R. Baer, S. Thevuthasan, V. Shutthanandan, M.H. Engelhard, C.H. Booth, and P. Nachimuthu. 2001. "The Structure of Na₂O-Al₂O₃-SiO₂ Glass: Impact on Sodium Ion Exchange in H₂O and D₂O." *Journal of Non-crystalline Solids* 296:10-26.

COLLABORATORS

Paul Tratnyek (Oregon Health and Sciences University); R. Lee Penn (University of Minnesota); You Qiang (University of Idaho); Dave Castner (University of Washington)

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EDUCATION

1991 B.S., Microbiology, Moscow State University, Russia

1992 M.S., Microbiology, Moscow State University, Russia

1999 Ph.D., Microbiology/Molecular Genetics, University of Massachusetts, Amherst

AREA OF EXPERTISE RELATED TO THIS PROJECT

Microbial physiology and genetics, microbial functional and comparative genomics, regulatory and gene network analysis using bioinformatics and experimental techniques.

PROFESSIONAL EXPERIENCE

1987 - 1992 Undergraduate and Graduate Student, Moscow State University, Moscow, Russia

- 1993 - 1995 Research Associate, Institute for Microbiology, Moscow, Russia
- 1995 - 1999 Graduate Teaching and Research Assistant, University of Massachusetts, Amherst, MA
- 1999 - 2002 Postdoctoral Research Associate, Oak Ridge National Laboratory, Oak Ridge, TN
- 2002 – present Senior Research Scientist, Pacific Northwest National Laboratory, Richland, WA

Ad Hoc Reviewer for Journals: Journal of Bacteriology, Applied & Environmental Microbiology, Environmental Microbiology, Environmental Science and Technology, Microbial Ecology, Microbiology, Canadian Journal of Microbiology.

AWARDS & SCHOLARSHIPS

- ORISE Fellowship Recipient, 1999-2002
- Student Travel Award, 7th International Conference on Small Genomes, 1999
- Graduate Assistant Fellowship, University of Massachusetts, 1995-1999
- International Undergraduate Exchange Program Scholarship, 1991-1992

PROFESSIONAL SOCIETIES

American Society for Microbiology: since 1997

SELECTED PUBLICATIONS (*Chronological Order*)

Pinchuk, G.E., C. Ammons, D.E. Culley, S.-M.W. Li, J.S. McLean, M.F. Romine, K.H. Nealson, J.K.

Fredrickson, and A.S. Beliae. 2007. " Utilization of DNA as a Sole Source of Phosphorus, Carbon, and Energy by *Shewanella*: Ecological and Physiological Implications for Dissimilatory Metal Reduction ". Appl. Environ. Microbiol. 2007 Dec 21; [Epub ahead of print].

Marshall, M.J., A.E. Plymale, D.W. Kennedy, L. Shi, Z. Wang, S.B. Reed, A.C. Dohnalkova, C.J. Simonson, C. Liu, D.A. Saffarini, M.F. Romine, J.M. Zachara, A.S. Beliae, and J.K. Fredrickson. 2007.

"Hydrogenase- and outer membrane c-type cytochrome-facilitated reduction of technetium(VII) by *Shewanella oneidensis* MR-1. Environ. Microbiol. Sep 20, 2007; [Epub ahead of print].

Bretschger, O., A. Obraztsova, C.A. Sturm, I.S. Chang, Y.A. Gorby, S.B. Reed, D.E. Culley, C.L. Reardon, S. Barua, M.F. Romine, J. Zhou, A.S. Beliae, R. Bouhenni, D. Saffarini, F. Mansfeld, B.H. Kim, J.K. Fredrickson, and K.H. Nealson. 2007. "An exploration of current production and metal oxide reduction by *Shewanella oneidensis* MR-1 wild type and mutants". Appl. Environ. Microbiol. 73:7003-7012.

- Elias, D.A., F. Yang, H.M Mottaz, A.S. Beliaev, and M.S Lipton. 2007. "Enrichment of Functional Redox Reactive Proteins and Identification by Mass Spectrometry Results in Several Terminal Fe(III)-reducing Candidate Proteins in *Shewanella oneidensis* MR-1". *J. Microbiol. Meth.* 68:367-375.
- Shi, L., M.U. Mayer, B. Chen, D.A. Elias, Y.A. Gorby, S. Ni, B.H. Lower, D.W. Kennedy, M.J. Marshall, E.A. Hill, A.S. Beliaev, J.M. Zachara, J.K. Fredrickson, and T.C. Squier. 2006. Isolation of a High-Affinity Functional Protein Complex between OmcA and MtrC: Two Outer Membrane Decaheme c-Type Cytochromes of *Shewanella oneidensis* MR-1. *J. Bacteriol.* 188: 4705-4714.
- Marshall, M.J., A.S. Beliaev, A.C. Dohnalkova, D.W. Kennedy, L. Shi, Z. Wang, M. Boyanov, B. Lai, K. M. Kemner, J.S. McLean, S.B. Reed, D.E. Culley, V.L. Bailey, C.J. Simonson, D.A. Saffarini, M.F. Romine, J.M. Zachara, J.K. Fredrickson. "The Role of *Shewanella oneidensis* MR-1 Outer Membrane c-Type Cytochromes in Uranium Reduction and Localization". *PLoS Biol.* 4(8): e268.
- Beliaev, A.S., D.M. Klingeman, J.A. Klappenbach, L. Wu, M.F. Romine, J.M. Tiedje, K.H. Nealson, J.K. Fredrickson, and J. Zhou. 2005. Global Transcriptome Analysis of *Shewanella oneidensis* MR-1 Exposed to Different Terminal Electron Acceptors. *J. Bacteriol.* 187:7138-7145.
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- Kolker, E., A.F. Picone, M.Y. Galperin, M.F. Romine, R. Higdon, K.S. Makarova, N. Kolker, G.A. Anderson, X. Qiu, K.J. Auberry, G. Babnigg, A.S. Beliaev et al. 2005. "Global Profiling of *Shewanella oneidensis* MR-1: Expression of 'Hypothetical' Genes and Improved Functional Annotations". *Proc. Natl. Acad. Sci. USA* 102(6):2099-2104
- Beliaev, A.S. 2004. Mutagenesis as a functional genomics tool. In Zhou, J., D. Thompson, Y. Xu, A. Beliaev, and J. Tiedje, *Microbial Functional Genomics*, pp. 207-240. John Wiley & Sons, New York, NY.
- Yost, C., L. Hauser, F. Larimer, D. Thompson, A. Beliaev, J. Zhou, Y. Xu, and D. Xu. 2003. A computational study of *Shewanella oneidensis* MR-1: Discovering the role of hypothetical proteins. *OMICS* 7(2): 177-192.
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- Liu, Y., J. Zhou, M. Omelchenko, A. Beliaev, A. Venkateswaran, J. Stair, L. Wu, D. K. Thompson, D. Xu, I. B. Rogozin, E. K. Gaidamakova, M. Zhai, K. S. Makarova, E. V. Koonin, and M. J. Daly. 2003. Transcriptome dynamics of *Deinococcus radiodurans* recovering from ionizing radiation. *Proc. Natl. Acad. Sci. USA* 100(7): 4191-4196.
- Beliaev, A., D. K. Thompson, D. A. Fields, M., L. Wu, D. P. Lies, K. H. Nealson and, J. Zhou. 2002. Microarray transcription profiling of a *Shewanella oneidensis* *etrA* mutant. *J. Bacteriol.* 184(16): 4612-4616.
- Beliaev, A., Thompson, D. K., C. Brandt, C. S. Giometti, D. P. Lies, K. H. Nealson and, J. Zhou. 2002. Gene and protein expression profiles of *Shewanella oneidensis* during anaerobic growth with different electron acceptors. *OMICS* 6(1): 39-60.
- Thompson, D. K., A. Beliaev, C. S. Giometti, D. P. Lies, K. H. Nealson, H. Lim, J. Yates III, J. Tiedje, and J. Zhou. 2002. Transcription and proteomic analyses of a ferric uptake regulator (*Fur*) mutant of *Shewanella oneidensis*: possible involvement of *Fur* in energy metabolism, regulation and oxidative stress. *Appl. Environ. Microbiol.* 68(2): 881-892.
- Phelps, T., A. V. Palumbo, and A. Beliaev. 2002. Metabolomics and microarrays for improved understanding of phenotypic characteristics controlled by both genomic and environmental constraints. *Curr. Opin. Biotechnol.* 13(1): 20-24.
- Beliaev, A., D. A. Saffarini, J. L. McLaughlin, and D. Hunnicut. 2001. MtrC, an outer-membrane decahaem c cytochrome required for metal reduction in *Shewanella putrefaciens* MR-1. *Mol. Microbiol.* 39(3): 722-730.

COLLABORATORS: Daad Saffarini (UWM), Igor Jouline (ORNL/UT), Frank Löffler (Georgia Tech), Robert Sanford (UIUC), Andrei Osterman (BIMR)

ANDREW R. FELMY

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EDUCATION

University of California, San Diego, Ph.D., 1988, Chemistry

University of Washington, M.S., 1981, Environmental Engineering

The Pennsylvania State University, B.S., 1977, Environmental Resource Management

EXPERIENCE

Dr. Felmy joined the Pacific Northwest National Laboratory (PNNL) in 1980 as a level I Scientist and has since been successively promoted to the highest scientific grade at the Laboratory, Level VI Laboratory Fellow. Dr. Felmy currently serves as The Chief Scientist for the Environmental Molecular Sciences Laboratory (EMSL) a National Scientific User Facility operated for the Department of Energy. Dr. Felmy's research interests are in the thermodynamics of aqueous and adsorption reactions in which he has been active for over 25 years. Dr. Felmy has authored more than 100 journal articles on the thermodynamics of aqueous and adsorption reactions with an emphasis on high-ionic-strength electrolytes and actinide species. Dr. Felmy has also been active in numerous professional societies and Department of Energy sponsored workshops in areas related to geosciences and electrolyte and actinide chemistry.

RELEVANT PROFESSIONAL ACTIVITIES

- Co-Organizer (with SB Clark) of the upcoming "MIGRATION 2009 - 12th International Conference on the Chemistry and Migration Behavior of Actinides and Fission Products in the Geosphere to be held at the Hanford site (current).
- Organized and chaired the Geosciences Session for the Office of Science/ORNL "Scientific Impacts and Opportunities in Computing" Workshop" (2008).
- Co-Chair (with KL Nagy) of the Chemical Migration Panel in the BES workshop "Basic Research Needs for Geosciences: Facilitating 21st Century Energy Systems (2007).
- Past Associate Editor of the Journal of Solution Chemistry.
- Served as the Hanford site coordinator for the Environmental Management Sciences Program in the area of High Level Waste (2003 – 2006).
- Organized the Environmental Molecular Sciences Laboratory Workshop "The Development of New User Research Capabilities in Environmental Molecular Science" (2006).
- Co-chaired (with RC Ewing) the Waste Chemistry and Materials Group at the Environmental Remediation Sciences Division 2nd Strategic Planning Workshop (2002).
- Co-organizer of the Mineral-Water Interface Symposium for the Environmental Molecular Sciences Laboratory (2002).
- Organized the ACS Symposium: Accomplishments of the Environmental Management Sciences Program (2001).
- Hosted the BES Geosciences Sixth Topical Research Symposium "Interfacial Processes in Geosciences"(1999)
- Served on the panel for the BES Chemical Sciences Heavy Element and Separation Science Program review of Argonne National Laboratory (1999).
- Chaired the BES Geosciences Research Program development of a Strategic Simulation Plan for modeling contaminant fate and transport in the subsurface (1998)

SELECTED PUBLICATIONS

- Rai D, DA Moore, AR Felmy, and H Bolton, Jr. 2007. "Environmental Mobility of Pu(IV) in the presence of ethylenediaminetetraacetic acid: Myth or Reality." *Radiochimica Acta* (in review).
- Felmy AR, HM Cho, DA Dixon, Y Xia, NJ Hess, and Z Wang. 2006. The Aqueous Complexation of Thorium with Citrate under Neutral to Basic Conditions. *Radiochimica Acta* 94(4):205-212
- Xia Y, NJ Hess, and AR Felmy. 2006. Stability Constants of Technetium (IV) Oxalate Complexes as a Function of Ionic Strength. *Radiochimica Acta* 94(3):137-141.
- Wang Z, AR Felmy, Y Xia, and EC Buck. 2006. Observation of Aqueous Cm(III)/Eu(III) and UO_2^{2+} Nanoparticulates at Concentrations Approaching Solubility Limit by Laser-Induced Fluorescence Spectroscopy. *Journal of Alloys and Compounds* 418(1-2):166-170.
- Cho HM, AR Felmy, RN Craciun, JP Keenum, NK Shah, and DA Dixon. 2006. Solution State Structure Determination of Silicate Oligomers by ^{29}Si NMR Spectroscopy and Molecular Modeling. *Journal of the American Chemical Society* 128(7):2324-2335.
- Ilton ES, C Liu, W Yantasee, Z Wang, DA Moore, AR Felmy, and JM Zachara. 2006. The Dissolution of Synthetic Na-Boltwoodite in Sodium Carbonate Solutions. *Geochimica et Cosmochimica Acta* 70(19):4836-4849.
- Felmy AR, Y Xia, and Z Wang. 2005. The Solubility Product of $\text{NaUO}_2\text{PO}_4 \cdot x\text{H}_2\text{O}$ Determined in Phosphate and Carbonate Solutions. *Radiochimica Acta* 93(7):401-408.
- Ilton ES, A Haiduc, CL Cahill, and AR Felmy. 2005. Mica Surfaces Stabilize Pentavalent Uranium. *Inorganic Chemistry* 44(9):2986-2988.
- Rai, D., N. J. Hess, M. Yui, A.R. Felmy, and D.A. Moore. 2004. "Thermodynamics and Solubility of $(\text{U}_x\text{Np}_{1-x})\text{O}_2(\text{am})$ Solid Solution in the Carbonate System." *Radiochimica Acta* 92:527-535.
- Xia, Y., A.R. Felmy, L. Rao, Z. Wang, and N.J. Hess. 2003. Thermodynamic Model for the Solubility of $\text{ThO}_2(\text{am})$ in the Aqueous $\text{Na}^+ - \text{H}^+ - \text{OH}^- - \text{NO}_3^- - \text{H}_2\text{O} - \text{EDTA}$ system. *Radiochimica Acta*, 91(12):751-760,
- Rai, D., D.A. Moore, A.R. Felmy, G.R. Choppin, and R.C. Moore. 2001. "Thermodynamics of the $\text{PuO}_2^+ - \text{Na}^+ - \text{OH}^- - \text{Cl}^- - \text{ClO}_4^- - \text{H}_2\text{O}$ System: Use of NpO_2^+ Pitzer Parameters for PuO_2^+ ." *Radiochimica Acta* 89:491-498.

PROFESSIONAL AFFILIATIONS

American Chemical Society

COLLABORATORS

Sue Clark (Washington State University), David Dixon (The University of Alabama), James Rustad (The University of California, Davis), John Weare (The University of California, San Diego), Paul Meakin (INL), Peter Lichtner (LANL), Gregory Choppin (Florida State University).

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EDUCATION

1971 B.S. in Microbiology, University of Illinois, Champaign, Illinois
1973 M.S. in Microbiology, University of Washington, Seattle, Washington
Ph.D. in Microbiology, University of Washington, Seattle, Washington

PROFESSIONAL EXPERIENCE

- Professor Emeritus, Purdue University, Dept. Biological Sciences (2007).
- Visiting Scientist, Biological Sciences Division, Pacific Northwest National Laboratory, Richland, Washington (2005).
- Erskine Fellow, Department of Civil Engineering, University of Canterbury, Christchurch, New Zealand. (2005).
- Sabbatical leave - Department of Microbiology, German National Research Centre for Biotechnology, Braunschweig, Germany (1992-1993).
- Professor, Purdue University, Dept. Biological Sciences (1992-2007).
- Visiting Associate Professor, Dept. Microbiology, University of Washington (Summer 1986).
- Sabbatical leave - Laboratory for Microbiology, University of Amsterdam, The Netherlands (1984-1985).
- Associate Professor, Purdue University, Dept. Biological Sciences (1983-1992).
- Assistant Professor, Purdue University, Dept. Biological Sciences (1977-1983).
- Postdoctoral Research Associate in the Department of Bacteriology, University of Wisconsin-Madison (1975-1977).

RESEARCH INTERESTS

- Physiological ecology of microbes in natural and engineered ecosystems
- Functional microbial community diversity
- Continuous culture of microorganisms.
- Soil microbial ecology
- Ecology of microbial heavy metal resistance in contaminated soils

PROFESSIONAL AFFILIATIONS

- Editorial Board, *Applied and Environmental Microbiology*, 1983-1994.
- Editorial Board, *Microbial Ecology*, 1995-
- Project director, Howard Hughes Medical Institute Program in Undergraduate Education, Department of Biological Sciences, Purdue University (2002-2007)
- Editorial Board, *Applied and Environmental Microbiology*, 2002-
- Erskine Fellow, University of Canterbury, 2005.
- Co-chair of 2010 International Society for Microbial Ecology Symposium (Seattle, WA)

AWARDS, HONORS, COMMITTEES

- Fulbright Scholar, 1984-1985.
- Fogarty Senior International Fellow, 1992-1993.
- Fellow, American Academy of Microbiology.

- National Science Foundation Ecology panel, 1996-2000.
- National Science Foundation Microbiology Postdoctoral Fellowship panel, 2001-2003.
- Carski Award Selection Committee, American Society for Microbiology, 2002-2005.

PUBLICATIONS (*Dr. Konopka has published over 100 journal articles and book chapters. Recent relevant publications are summarized below*)

- Blume, E., Bischoff, M., Reichert, J.M., Moorman, T., Konopka, A. and Turco, R.F. (2002) Surface and subsurface microbial biomass, community structure and metabolic activity as a function of soil depth and season. *Appl. Soil. Ecol.* 20: 171-181.
- Shi, W., Bischoff, M., Turco, R. and Konopka, A. 2002. Association of microbial community composition and activity with Pb, Cr and hydrocarbon contamination. *Appl. Environm. Microbiol.*, 68(8): 3859-3866.
- Konopka, A., Zakharova, T. and Nakatsu, C.N. 2002. Effect of starvation length upon lags in substrate degradation in a biomass recycle reactor. *J. Industr. Microbiol. Biotech* 29(5): 286-291.
- LaPara TM, Zakharova T, Nakatsu CH, and Konopka, A. 2002. Functional and structural adaptations of bacterial communities growing on particulate substrates under stringent nutrient limitation *Microbial Ecol* 44 (4): 317-326.
- Konopka, A. 2004. Systems biology – not brand new, but different. *ASM News* 70(4) 163-168.
- Young, J., Henne, K., Morgan, J., Konopka, A. and Ramkrishna, D. 2004. Cybernetic modeling of metabolism: towards a framework for rational design of recombinant organisms *Chemical Engineering Science* 59: 5041-5049
- Shi, W., Bischoff, M., Turco, R.F. and Konopka, A. 2005. Microbial catabolic diversity in soils contaminated with hydrocarbons and heavy metals. *Environm Sci Technol* 39: 1974-1979.
- Becker, J.M., Parkin, T., Nakatsu, C.H., Wilbur, J.D., and Konopka, A. 2006. Bacterial activity, community structure, and cm-scale spatial heterogeneity in contaminated soil. *Microb. Ecol.* 50: 220-231.
- Joynt, J. Bischoff, M., Turco, R., Konopka, A. and Nakatsu, C.H. 2006. Microbial community analysis of soils contaminated with lead, chromium and petroleum hydrocarbons. *Microb. Ecol.* 51: 209-219.
- Nakatsu, C.H., Carmosini, N., Baldwin, B., Beasley, F., Kourtev, P. and Konopka, A. 2005. Soil microbial community responses to additions of organic carbon substrates and heavy metals (Pb and Cr). *Appl. Environm. Microbiol.* 71: 7679-7689.
- Kourtev, P. S., C. H. Nakatsu, and Konopka, A. 2006. Anaerobic bacterial community responses to organic C addition in chromium (VI) and iron (III) amended microcosms. *Applied And Environmental Microbiology* 72: 628-637.
- Carrero-Colon M, Nakatsu CH, and Konopka A. 2006. Microbial community dynamics in nutrient-pulsed chemostats. *FEMS Microbiology Ecology* 57: 1-8.
- Vargha, M., Takats, Z, Konopka, A and Nakatsu CH. 2006. Optimization of MALDI-TOF MS for strain level differentiation of *Arthrobacter* isolates. *J. Microbiol. Methods* 66: 399-409.
- Carrero-Colon M, Nakatsu CH, and Konopka A. 2006. The effect of nutrient periodicity upon microbial community dynamics. *Appl. Environm. Microbiol.*, 72: 3175-3183.
- Konopka, A. 2006. Microbial ecology: searching for principles. *Microbe* 1: 175-179.
- Carrero-Colon M, Nakatsu CH, and Konopka A. 2007. Community dynamics and heterogeneities in mixed bacterial communities subjected to nutrient periodicities. *Environm. Microbiol.* 9: 1584-1590.
- Hill, K. A., P. B. Shepson, E. S. Galbavy, C. Anastasio, P. S. Kourtev, A. Konopka, and B. H. Stirm (2007), Processing of atmospheric nitrogen by clouds above a forest environment, *J. Geophys. Res.*, 112, D11301, doi:10.1029/2006JD008002.

COLLABORATORS

Purdue University: Doerge, Rebecca W.; Nakatsu, Cindy H.; Ramkrishna, Doraiswami; Thompson, Dorothea; Turco, Ron

Other Institutions: Fredrickson, J. (PNNL); LaPara, T. (U. of Minnesota); Staley, J.T. (U. of Washington)

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EDUCATION

Ph.D. - Johns Hopkins University, Baltimore, Maryland, 1994-1998, Environmental Engineering and Chemistry
M.S. - University of Alabama, Tuscaloosa, Alabama, 1992-1994, Aqueous Geochemistry
M.S.E. - Zhejiang University, Hangzhou, China, M.S.E., 1982-1984, Hydrology and Hydrogeochemistry
B.S. - Zhejiang University, Hangzhou, China, 1978-1982, Geology

PROFESSIONAL EXPERIENCE

2000-present, Level III, IV, and V Scientist, Pacific Northwest National Laboratory
1998-2000 Postdoctoral Fellow, Pacific Northwest National Laboratory
1988-1991 Lecturer, Ningbo University, China
1984-1988 Engineer, Zhejiang Hydrology and Hydropower Design Institute, China

RESEARCH EXPERIENCE AND INTEREST

Dr. Liu's research area is in the geochemistry and biogeochemistry with a focus on the solute and contaminant mass transfer and biogeochemical modeling in subsurface environments. His researches typically employ: 1) laboratory experiments (e.g., batch and column) or field systems to derive macroscopic reaction networks, and phenomenological rates of reaction and diffusive mass transfer for model characterization and validation; 2) various microscopic and spectroscopic techniques, and molecular simulation tools to provide microscopic and molecular insights on process pathways and rate expressions; and 3) mathematical models at relevant scales for data interpretation, concept validation, and projection. His recent research areas include: a) theoretical and experimental investigations of microscopic reactive diffusion from molecular to pore scales, b) coupled diffusion and biogeochemical reactions and their control on uranium and technetium fate and transport in subsurface sediments, and c) scaling of biogeochemical reactions and diffusive mass transfer from microscopic to large and field scale.

PROFESSIONAL AFFILIATIONS

American Geophysical Union
American Chemical Society
Geological Society of America

SELECT RECENT PUBLICATIONS (*from over 50*)

- Liu C, Zachara, JM, Foster-Mills NS, Strickland J., 2007, Kinetics of reductive dissolution of hematite by bioreduced anthraquinone-2,6-disulfonate, *Environ. Sci. Technol.*, 41 7730-7735.
- Kerisit SN, Liu C, and Ilton ES, 2008, Molecular dynamics simulations of the orthoclase (001)- and (010)-water interfaces, *Geochim. Cosmochim. Acta*, in press.
- Liu C, Zachara JM, Jeon B-H, Wang Z., Dohnalkova A., and Fredrickson, JK, 2007, Influence of calcium on microbial reduction of solid phase U(VI), *Biotech. Bioeng.*, 97, 1415-1422.
- Liu C, 2007, An ion diffusion model in semi-permeable clay materials, *Environ. Sci. Technol.*, 41, 5403-5409.

- Fang J, Gu Z, Gand D, Liu C, Ilton ES, and Deng B, 2007, Cr(VI) Removal from Aqueous Solution using a Commercial Activated Carbon Coated with Quaternized poly(4-vinylpyrriene), *Environ. Sci. Technol.*, 41, 4748-4753.
- Marshall MJ, Plymale AE, Kennedy DW, Shi L, Wang Z, Reed SB, Dohnalkova AC, Simonson CJ, Liu C, Saffarini DA, Romine MF, Zachara JM, Beliaev AS, and Fredrickson JK, 2008, Biomolecular mechanisms of Tc(IV)O₂ nanoparticle formation by *Shewanella oneidensis* MR-1: A novel technetium(VII) reductase activity by c-type cytochromes., *Environ. Microbiol.*, in press
- Liu C, and Ball WP, 2008, Application of the Generalized Integral Transform Technique for Solute Transport Modeling in Heterogeneous Porous Media in HYBRID METHODS IN ENVIRONMENTAL CONTAMINANT DISPERSION (ed. Cotta et al.), in press.
- Ilton ES, Qafoku N, Liu C, Moore D, and Zachara JM, 2008, Advective removal of intraparticle uranium from contaminated vadose zone sediment, Hanford, USA, *Environ. Sci. Technol.*, in press.
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- Ilton ES, Heald SM, Smith SC, Elbert D, and Liu C, 2006, Reduction of uranyl in the interlayer region of low iron micas under anoxic and aerobic conditions, *Environ. Sci. Technol.*, 40, 5003-5009.
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COLLABORATORS

John Zachara (PNNL), James Fredrickson (PNNL), James McKinley (PNNL), Jack Istok (Oregon State University), Baolin Deng (University of Missouri-Columbia), Hailiang Dong (University of Miami, OH), William Ball (Johns Hopkins University).

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EDUCATION

1998 Ph.D. Geochemistry; Virginia Polytechnic Institute and State University

1994 M.S. Geochemistry; Virginia Polytechnic Institute and State University

1992 B.S. Geochemistry; California State Polytechnic University, Pomona

EXPERIENCE

Dr. Rosso is a Staff Scientist and Associate Director for the Chemical and Materials Sciences Division. His research is centered on elucidating the relationships between the atomic and electronic structure of crystalline materials with their reactivity and physical properties, particularly at interfaces, using various concepts and tools of surface science, chemistry, solid state physics, and crystal chemistry. His recent research is focused on unraveling rates and mechanisms of biogeochemical electron transfer towards a better understanding of subsurface contaminant transport. Dr. Rosso has published 75 peer-reviewed publications and several book chapters on various aspects of mineral/water and mineral/microbe interface chemistry.

EMPLOYMENT

3/06 – Present Associate Director - Environmental Dynamics and Simulation, PNNL

1/05 – 2/06 Staff Scientist - Environmental Dynamics and Simulation, PNNL

1/02 – 12/04 Senior Research Scientist II - Environmental Dynamics and Simulation, PNNL

1/00 - 12/01 Senior Research Scientist I - Environmental Dynamics and Simulation, PNNL

6/98 - 12/99 Research Scientist - Environmental Dynamics and Simulation, PNNL

DISTINCTIONS AND SERVICE

- The 2004 Mineralogical Society of America Award
- The Laboratory Director's Award - Pacific Northwest National Laboratory, 2004
- Nominated for the U.S. Presidential Early Career Scientist and Engineer Award
- Associate Editor - American Mineralogist (2004-2006)
- Organized six topical symposia for Goldschmidt and American Chemical Society national meetings

SELECTED PUBLICATIONS

Wigginton, N.S., Rosso K.M., and Hochella M.F. (2007) Mechanisms of electron transfer in two decaheme cytochromes from a metal-reducing bacterium. *Journal of Physical Chemistry B* 111: 12857-12864.

Wigginton N.S., Rosso K.M., Lower B.H., Shi L., and Hochella M.F. (2007) Electron tunneling properties of outer-membrane decaheme cytochromes from *Shewanella oneidensis*. *Geochimica et Cosmochimica Acta* 71(3):543-555.

Wander M.C., Rosso K.M., and Schoonen M.A. (2007) Structure and charge hopping dynamics in green rust. *Journal of Physical Chemistry C* 111(30):11414-11423.

Kerisit S.N., Rosso K.M., Dupuis M., and Valiev M. (2007) Molecular computational investigation of electron transfer kinetics across cytochrome-iron oxide interfaces. *Journal of Physical Chemistry C* 111(30):11363-11375.

- Kerisit S.N., and Rosso K.M. (2007) Kinetic Monte Carlo model of charge transport in hematite (α -Fe₂O₃). *Journal of Chemical Physics* 127(12):124706.
- Droubay T.C., Rosso K.M., Heald S.M., McCreedy D.E., Wang C.M., and Chambers S.A. (2007) Structure, magnetism and conductivity in epitaxial Ti-doped α -Fe₂O₃ hematite: Experiment and density functional theory calculations. *Physical Review B, Condensed Matter and Materials Physics* 75(10):104412.
- Deskins N.A., Kerisit S.N., Rosso K.M., and Dupuis M. (2007) Molecular dynamics characterization of rutile-anatase interfaces. *Journal of Physical Chemistry C* 111(26):9290-9298.
- Chambers S.A., Droubay T.C., Wang C.M., Rosso K.M., Heald S.M., Schwartz S.A., Kittilstved K.R., and Gamelin D.R. (2006) Ferromagnetism in oxide semiconductors. *Materials Today* 9(11):28-35.
- Kerisit S. and K.M Rosso (2006) "Computer simulation of electron transfer at hematite surfaces." *Geochimica et Cosmochimica Acta* 70:1888-1903.
- Rosso K.M. and Vaughan D.J. (2006) Sulfide mineral surfaces. In *Mineralogy and Geochemistry of Sulfides*. Reviews in Mineralogy and Geochemistry, 61, 505-556, Mineralogical Society of America.
- Rosso K.M. and Vaughan D.J. (2006) Reactivity of sulfide mineral surfaces. In *Mineralogy and Geochemistry of Sulfides*. Reviews in Mineralogy and Geochemistry, 61, 557-607, Mineralogical Society of America.
- Gorby Y. A., Yanina S., McLean J. S., Rosso K. M., Moyles D., Dohnalkova A., Beveridge T. J., Chang I. S., Kim B. H., Kim K. S., Culley D. E., Reed S. B., Romine M. F., Saffarini D. A., Hill E. A., Shi L., Elias D. A., Kennedy D. W., Pinchuk G., Watanabe K., Ishii S., Logan B., Nealson K. H., and Fredrickson J. K. (2006) Electrically conductive bacterial nanowires produced by *Shewanella oneidensis* strain MR-1 and other microorganisms. *Proceedings of the National Academy of Sciences of the United States of America* 103(30), 11358-11363.
- Rosso K.M., and Dupuis M. (2006) "Electron transfer in environmental systems: A frontier for theoretical chemistry." *Theoretical Chemistry Accounts* 116(1-3):124-136.
- Smith D.M., K.M. Rosso, M. Dupuis, M. Valiev, and T. Straatsma (2006) "Electronic coupling between heme electron-transfer centers and its decay with distance depends strongly on relative orientation." *Journal of Physical Chemistry B* 110(31):15582-15588.
- Yanina S.V., K.M. Rosso, and P. Meakin (2006) "Defect distribution and dissolution morphologies on low-index surfaces of α -quartz." *Geochimica et Cosmochimica Acta* 70:1113-1127.
- Wander M.C.F., Kerisit S., Rosso K.M., and Schoonen M. A. A. (2006) Kinetics of triscarbonate uranyl reduction by aqueous ferrous iron: A theoretical study. *Journal of Physical Chemistry A* 110(31), 9691-9701.
- Neal A.L., Bank T.L., Hochella M.F., and Rosso K.M. (2005) Cell adhesion of *Shewanella oneidensis* to iron oxide minerals: Effect of different single crystal faces. *Geochemical Transactions* 6(4), 77-84.
- Rosso K.M., Smith D.M.A., and Dupuis M. (2004) Aspects of iron and manganese self-exchange electron transfer reactions. *Journal of Physical Chemistry A*, 108, 5242-5248.
- Rosso K.M., Zachara J.M., Fredrickson J.K., Gorby Y.A., and Smith S.C. (2003) Non-local bacterial electron transfer to hematite surfaces. *Geochimica et Cosmochimica Acta*, 67, 1081-1087.
- Rosso K.M., Smith D.M.A., Dupuis, M. (2003) An ab initio model of electron transport in hematite (α -Fe₂O₃) basal planes. *Journal of Chemical Physics*, 118, 6455-6466.

COLLABORATORS

Paul Meakin (Idaho National Lab); Gordon Brown (Stanford University); Michael Hochella (Virginia Tech); Gerald Gibbs (Virginia Tech); Paul Fenter (Argonne); Jeff Catalano (Washington University); Michelle Scherer (University of Iowa); Rod Ewing (Michigan); Martin Schoonen (Stony Brook)

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EDUCATION

1993 Ph.D., civil engineering, Stanford University
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EXPERIENCE

Pacific Northwest National Laboratory (1992-Present)
1992-1995: Research Scientist
1996-1999: Senior Research Scientist I
2000-2002: Senior Research Scientist II
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Dr. Scheibe joined Pacific Northwest National Laboratory in September 1992. At PNNL, he has been responsible for proposal development, project management, and technical contributions in a number of different areas of environmental research and technology development broadly related to the hydrologic sciences. His primary research focus is on characterization and modeling of natural subsurface heterogeneity and its impacts on reactive transport in groundwater systems. His research projects include both computational and field experimental elements. Recently, he has worked on problems in the area of subsurface biogeochemistry, including microbial transport in groundwater and bioremediation of metals and radionuclides. He is currently collaborating with computational scientists, biologists, and applied mathematicians to simulate coupled flow, transport, and biogeochemical processes at cellular, pore and continuum scales. His research is supported primarily by the Department of Energy's Office of Science through the Environmental Remediation Science Program (ERSP) and the Scientific Discovery through Advanced Computing (SciDAC) program. Dr. Scheibe serves on the editorial board of the journal *Ground Water*. He is an active member of the American Geophysical Union and is currently serving as chairperson of the Groundwater Technical Committee, Outstanding Student Presentation Award co-coordinator for the Fall Meeting, and Hydrology Section Program Chair for the Spring Meeting (Joint Assembly). Dr. Scheibe has authored or co-authored 27 articles in peer-reviewed scientific journals; selected publications of particular relevance are listed below:

PUBLICATIONS

- Kamolpornwijit, W., S. C. Brooks, Y.-J. Kim, and T. D. Scheibe, "A Novel Approach to Estimate the Distribution of Reducible Iron Oxides Within Different Pore Domains of Structured Media," *Applied Geochemistry* 22(12): 2630-2636, 2007.
- Tartakovsky, A. M., P. Meakin, T. Scheibe, and B. D. Wood, "A smoothed particle hydrodynamics model for reactive transport and mineral precipitation in porous and fractured porous media," *Water Resources Research*, 43(5): Art. No. W05437, doi:10.1029/2005WR004770, 2007.
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- Scheibe, T. D. and C. R. Cole, "Non-Gaussian particle tracking: Application to scaling of transport processes in heterogeneous porous media", *Water Resources Research*, 30(7):2027-2039, 1994.

COLLABORATORS

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EDUCATION

1996 Ph.D. Biomedical Science; Hauzhong Agricultural Univ.-P. R. China

1985 M.S. Plant Pathology; Hauzhong Agricultural Univ.-P. R. China

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EXPERIENCE

1985-88 Lecturer, Hauzhong Agricultural University-P. R. China

1988-90 Visiting Scholar, Ohio State University-Columbus/OH

1999-2002 Research Associate, Case Western Reserve University-Cleveland/OH

2002-06 Senior Research Scientist I, Pacific Northwest National Lab.-Richland/WA

2007-Present Senior Research Scientist II, Pacific Northwest National Lab.-Richland/WA

PROFESSIONAL SOCIETIES

American Society for Microbiology

American Society for Biochemistry and Molecular Biology

PUBLICATIONS (of total 35)

CM Eggleston, J Voros, L Shi, BH Lower, TC Droubay and PJS Colberg. 2008. Binding and direct electrochemistry of OmcA, an outer-membrane cytochrome from an iron reducing bacterium, with oxide electrodes: A candidate biofuel cell system. *Inorganica Chimica Acta*. (in press, doi:10.1016/j.ica.2007.07.015).

MJ Marshall, AE Plymale, DW Kennedy, L Shi, Z Wang, S Reed, A Dohnalkova, CJ Simonson, C Liu, D Saffarini, MF Romine, JM Zachara, AS Beliaev and JK Fredrickson. 2008. Hydrogenase- and outer membrane *c*-type cytochrome-facilitated reduction of technetium (VII) by *Shewanella oneidensis* MR-1. *Environmental Microbiology*. 10: 125-136.

RS Hartshorne RS, BN Jepson, TA Clarke, SJ Field, JK Fredrickson, J Zachara, L Shi, JN Butt and DJ Richardson. 2007. Characterization of *Shewanella oneidensis* MtrC: a cell surface decaheme cytochrome involved in respiratory electron transport to extracellular electron acceptors. *Journal of Biological Inorganic Chemistry*.12: 1083-1094.

L Shi, TC Squier, JM Zachara and JK Fredrickson. 2007. Respiration of metal (hydr)oxides by *Shewanella* and *Geobacter*: a key role for multiheme *c*-type cytochromes. *Molecular Microbiology*. 65: 12-20.

NS Wigginton, KM Rosso, BH Lower, L Shi and MF Hochella, Jr. 2007. Electron tunneling properties of outer-membrane decaheme cytochromes from *Shewanella oneidensis*. *Geochimica et Cosmochimica Acta*. 71: 543-555.

BH Lower, L Shi, R Yongsunthon, TC Droubay, DE McCready, and SK Lower. 2007. Dynamic force spectroscopy of specific bonds that form between an iron oxide surface and outer membrane cytochromes OmcA and MtrC from *Shewanella oneidensis*. *Journal of Bacteriology* 189: 4944-4952.

Y Xiong, L Shi, B Chen, MU Mayer, S Bose, MF Hochella, JK Fredrickson, and TC Squier. 2006. High-affinity binding and direct electron transfer to solid metals by purified metal reducing protein OmcA decaheme cytochrome. *Journal of the American Chemical Society*. 128: 13978-13979.

L Shi, B Chen, Z Wang, DA Elias, MU Mayer YA Gorby, S Ni, BH Lower, DW Kennedy, DS Wunschel, HM Mottaz, MJ Marshall, EA Hill, AS Beliaev, JM Zachara, JK Fredrickson and TC Squier. 2006. Isolation of a high-affinity functional protein complex between OmcA and MtrC: two decaheme *c*-type cytochromes of *Shewanella oneidensis* MR-1. *Journal of Bacteriology*. 188: 4705-4714.

- MJ Marshall, AS Beliaev, AC Dohnalkaova, DW Kennedy, L Shi, Z Wang, MI Boyanov, B Lai, KM Kemner, JS Mclean, SB Reed, DE Culley, VL Bailey, CJ Simonson, DA Saffarini, MF Romine, JM Zachara and JK Fredrickson. 2006. *c*-Type cytochrome-dependent formation of U(IV) nanoparticles by *Shewanella oneidensis*. *PLoS Biology*. 4: 1324-1333.
- YA Gorby, S Yanina, JS McLean, KM Rosso, D Moyles, A Dohnalkova, TJ Beveridge, IS Chang, A Korenevski, BH Kim, KS Kim, DE Culley, SB Reed, MF Romine, DA Saffarini, EA Hill, L Shi, DA Elias, DW Kennedy, G Pinchuk, K Watanabe, S Ishii, B Logan, KH Nealson and JK Fredrickson. 2006. Electrically conductive bacterial nanowires produced by *Shewanella oneidensis* strain MR-1 and other microorganisms. *Proceedings of National Academy of Science USA*. 103:11358-11363.
- W Zhang and L Shi. 2005. Distribution and evolution of multiple-step phosphorelay in prokaryotes: lateral domain recruitment involved in the formation of hybrid-type histidine kinases. *Microbiology* 151: 2159-2173.
- R Li, MB Potters, L Shi and PJ Kennelly. 2005. The protein phosphatases of *Synechocystis* sp. strain PCC 6803: open reading frames sll1033 and sll1387 encode enzymes that exhibit both protein-serine and protein-tyrosine phosphatase activity in vitro. *Journal of Bacteriology*. 187: 5877-5884.
- UU Mayer-Cumblidge, L Shi and TC Squier. 2005. One-step, non-denaturing pull-down of an RNA polymerase core enzyme complex using an improved multi-affinity probe resin. *Molecular BioSystems* 1: 53-56.
- L Shi, J-T Lin, LM Markillie, TC Squier and BS Hooker. 2005. Over-expression of multi-heme *c*-type cytochromes. *BioTechniques* 38: 297-299.
- LM Markillie, J-T Lin, JN Adkins, DL Auberry, E Hill, BS Hooker, PA Moore, RJ Moore, L Shi, S Wiley and V Kery. 2005. A simple protein complex purification and identification method for high throughput mapping of protein interaction networks. *Journal of Proteome Research* 4: 268-274.
- F Yang, B Bogdanov, EF Strittmatter, AN Vilkov, MA Gritsenko, L Shi, DA Elias, S Ni, MF Romine, L Pasatolic, MS. Lipton and RD Smith. 2005. Characterization of purified *c*-type heme-containing peptides and identification of *c*-type heme-attachment sites in *Shewanella oneidensis* cytochromes using mass spectrometry. *Journal of Proteome Research* 4: 846-854.
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- L Shi and W Zhang. 2004. Comparative analysis of eukaryotic-type protein phosphatases in two streptomycete genomes. *Microbiology* 150: 2247-2256.
- L Shi. 2004. Manganese-dependent protein O-phosphatases in prokaryotes and their biological functions. *Frontiers in Bioscience* 9:1382-1397.
- L Shi, DG Kehres and ME Maguire. 2001. The PPP-family protein phosphatases PrpA and PrpB of *Salmonella enterica* serovar Typhimurium possess distinct biochemical properties. *Journal of Bacteriology* 183:7053-7057
- L Shi, KM Bischoff and PJ Kennelly. 1999. The *IcfG* gene cluster of *Synechocystis* sp PCC6803 encodes an Rsb/Spo-like protein kinase, protein phosphatase, and two phosphoproteins. *Journal of Bacteriology* 181: 4761-4767.
- L Shi, WW Carmichael and PJ Kennelly. 1999. Cyanobacterial PPP-family protein phosphatases possess multifunctional capabilities and are resistant to microcystin-LR. *Journal of Biological Chemistry* 274: 10039-10046.
- L Shi, M Potts and PJ Kennelly. 1998. The serine, threonine, and/or tyrosine-specific protein kinases and protein phosphatases of prokaryotic organisms: a family portrait. *FEMS Microbiology Reviews* 22: 229-253.
- KM Bischoff, L Shi and PJ Kennelly. 1998. The detection of enzyme activity following SDS-polyacrylamide gel electrophoresis. *Analytical Biochemistry* 260: 1-17.

COLLABORATORS

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EDUCATION

University of Guelph, Ph.D., 1993, Soil Physics
University of Guelph, M.Sc., 1989, Soil Science
University of the West Indies, B.Sc. (1st Class Hons), 1986, Agricultural Science

EXPERIENCE

Dr. Ward has performed extensive experimental studies of field-scale flow and transport processes in the vadose zone with a focus on multi-scale characterization methods for heterogeneous soils. His research encompasses both basic and applied components and has ranged from fundamental studies of the effect of pore-scale heterogeneities and morphology on hydraulic properties to the joint inversion of field-scale flow and transport data sets with large parameter dimension. Dr. Ward's current research is focused on the development of a theoretical framework for building 3D geological models of unconsolidated sediments and populating the simulation grid with appropriately upscaled parameters using geophysical data constraints. His research is assisted by applications of electron microscopy, nuclear magnetic resonance, x-ray diffraction, geophysics (time domain reflectometry, radar, and resistivity) to the characterization of porous media.

PROFESSIONAL AFFILIATIONS

- American Geophysical Union
- International Association of Mathematical Geology
- National Association of Black Geologists and Geophysicists
- Soil Science Society of America

RELEVANT PROFESSIONAL ACTIVITIES

- Lead scientist for vadose zone hydrology task of the Remediation and Closure Science Project at the U.S Department of Energy Hanford Site (2004 to present)
- Past associate editor of the Soil Science Society of America Journal
- Co-lead (with Dr. Glendon Gee) of the Vadose Zone Transport Field Studies of the Science and Technology at the U.S Department of Energy Hanford Site (1999 to 2004)
- Adjunct professor, Civil and Environmental Engineering, Washington State University, Tri-cities.

SELECTED PUBLICATIONS

- Clement WP, and AL Ward. 2008. "Using Ground Penetrating Radar to Measure Soil Moisture Content." Book Title: *Handbook of Agricultural Geophysics*. Editors: BJ Allred, JJ Daniels, and M Reza Ehsani, CRC Press (4/25/2008 Publication Date).
- Ward AL, and ZF Zhang. 2007. Effective Hydraulic Properties Determined from Transient Unsaturated Flow in Anisotropic Soils. *Vadose Zone J.* 6:913–924
- Ward AL. 2007. A Comparison of Upscaling Methods for Predicting Flow in Highly Heterogeneous, Anisotropic Sediments. *Vadose Zone J.* (*Accepted*)
- Conrad ME, DJ DePaolo, K Maher, GW Gee, and AL Ward. 2007. Field Evidence for Strong Chemical Separation of Contaminants in the Hanford Vadose Zone. *Vadose Zone J.* 6: 1031–1041.
- Murray CJ, AL Ward, and J Wilson. 2007. Influence of Clastic Dikes on Vertical Migration of Contaminants at the Hanford Site. *Vadose Zone J.* 6: 959–970

- Tartakovsky, AM, P Meakin, and AL Ward. 2007. Smooth Particle Hydrodynamics Model of NAPL Flow and Dissolution, *Transport in Porous Media (In Press)*
- Tartakovsky AM, AL Ward and PM Meakin. 2007. Pore-scale simulations of drainage of heterogeneous and anisotropic porous media. *Physics of Fluids*, 19(10):103301-103301-8.
- Zhang ZF, M Oostrom, and AL Ward. 2007. Saturation-Dependent Hydraulic Conductivity Anisotropy for Multifluid Systems in Porous Media. *Vadose Zone J* 6:925–934.
- Stewart ML, AL Ward, DR Rector. 2006. Study of Pore Geometry Effects on Anisotropy in Hydraulic Permeability Using the Lattice-Boltzmann Method. *Advances in Water Resources* 29(9): 1328-1340.
- Ward AL, ZF Zhang, and GW Gee. 2006. Upscaling unsaturated hydraulic parameters for flow through heterogeneous anisotropic sediments. *Adv. in Water Resour.* 29:268-280.
- Kowalsky MB, SA Finsterle, JE Peterson, S Hubbard, Y Rubin, EL Majer, AL Ward, and GW Gee. 2005. Estimation of field-scale soil hydraulic and dielectric parameters through joint inversion of GPR and hydrological data. *Water Resour. Res.*, 41:W11425, doi:10.1029/2005WR004237
- Seedahmed GH, and AL Ward. 2005. Scale-Space Mutual Information for Textural-Patterns Characterization. ACTA Press. (<http://www.actapress.com/PaperInfo.aspx?PaperID=21370>)
- Zhang ZF, AL Ward, and GW Gee. 2004. A combined parameter scaling and inverse technique to upscale the unsaturated hydraulic parameters for heterogeneous soils. *Water Resour. Res.* 40(8), W08306, doi:10.1029/2003WR002925.
- Zhang ZF, AL Ward, and GW Gee. 2004. A parameter scaling concept for estimating field-scale hydraulic functions of layered soils. *Journal of Hydraulic Research*, 41(extra):93-103.
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- Zhang ZF, AL Ward, and GW Gee. 2003. Estimating Soil Hydraulic Parameters of a Field Drainage Experiment Using Inverse Techniques. *Vadose Zone Journal* 2:201-211.
- Gee, GW, AL Ward, and ZF Zhang, GS Campbell, and J Mathison. 2002. The influence of hydraulic non-equilibrium on pressure plate data. *Vadose Zone Journal*, 1:172-178.
- Yabusaki SB, and AL Ward. 2004. High-Resolution Modeling Studies of Vadose Zone Reactive Transport. (Invited Paper No. 217-7) *Geological Society of America Abstracts with Programs.* 35(6):531, September 2003.
- Ward AL, ZF Zhang, JM Keller, and ZF Zhang. 2004. Hydrostratigraphic Characterization Using High-resolution Borehole Moisture Logs and Grain-size Distribution Statistics Fall Meet. Suppl., Abstract H23A- H23A-1110.
- Fink JB, AL Ward, GW Gee. 2001. “Vadose Zone Injection Monitoring with Electrical Geophysics Using Steel Casings as Electrodes.” AGU Fall Meetings, San Francisco, CA, December 5-9, 2001
- Zhang ZF, AL Ward, GW Gee, MD White. 2002. “Parameter Estimation for Unsaturated Layered Soils Through a Combination of Non-similar Media Scaling and Inverse Flow Modeling.” IAHR International Groundwater Symposium "Bridging the Gap between Measurement and Modeling in Heterogeneous Media," International Groundwater Symposium, Berkeley, CA, March 25-28, 2002.

COLLABORATORS

Roelof Versteeg (INL); Andrew Binley (Lancaster University)

STEVEN D. CONRADSON

XAFS Project Leader

Structure/Function Relations Group, Material Science and Technology Division

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EDUCATION

Stanford University, Ph.D., 1983, Physical Chemistry

Harvard University, NIH Postdoctoral Fellowship

San Jose State University, B.S., 1977, Chemistry

EXPERIENCE

Dr. Conradson has been characterizing local structure and chemical speciation using synchrotron x-ray methods for 30+ years, and is best known for the early identification of local lattice defects in cuprates and for pioneering the routine application of synchrotron radiation to transuranic-containing materials. He has also recently extended this experimental program to modeling lattice distortions, cooperative phenomena, and nanoscale heterogeneity in complex materials. Scientific interests include the application of synchrotron x-rays to the materials science, chemistry, and environmental chemistry of transuranic elements, as well as the area of lattice distortions and structure:property relationships in complex functional materials. Specific topics include bioinorganic chemistry, low dimensional materials, cuprate superconductors and manganites, actinide chemistry and materials science, electronic structure methodology, magnetic materials, catalysis, time resolved x-ray absorption, x-ray absorption theory, structural analysis and other local approaches to nanoscale heterogeneity.

PROFESSIONAL AFFILIATIONS

- American Chemical Society
- American Association for the Advancement of Science
- Materials Research Society

RELEVANT PROFESSIONAL ACTIVITIES

- Organizer, Local and Nanoscale Structure in Complex Systems, 2002
- Organizer, Dynamic Energy Landscapes and Functional Systems, 2004
- Organizer, Materials R&D for National Security at DOE User Facilities; Determining Structure:Function Relationships in Security-Relevant Materials, 2005
- Organizer, DELFS III, Organization and Cooperative Phenomena in Condensed Matter and Biomolecules.

SELECTED HONORS AND AWARDS

2000 Los Alamos National Laboratory Distinguished Performance Award – XAFS of PuGa Alloys

1995 Pacific Northwest National Laboratory – Speciation in Hanford Tank Wastes

SELECTED PUBLICATIONS AND INVITED PRESENTATIONS

Over 90 publications in refereed journals, including Science, Physical Review Letters, and Journal of the American Chemical Society, several of which have garnered more than 100 citations, and over 70 conference presentations on an exceptionally wide range of subjects.

- Conradson, S. D.; Burgess, B. K.; Newton, W. E.; Mortenson, L. E.; Hodgson, K. O. 1987. Structural Studies of the Molybdenum Site in the MoFe Proteins and its FeMo Cofactor by EXAFS, *J. Amer. Chem. Soc.* (109) 7507-7515.
- de Leon, J. M.; Conradson, S. D.; Batistic, I.; Bishop, A. R. 1990. Evidence for an Axial Oxygen-Centered Lattice Fluctuation Associated with the Superconducting Transition in $\text{YBa}_2\text{Cu}_3\text{O}_7$, *Phys. Rev. Lett.* (65) 1675-1678
- Conradson, S. D.; Raistrick, I. D.; Bishop, A. R. 1990. Axial Oxygen-Centered Lattice Instabilities and High-Temperature Superconductivity, *Science* 1248 1394-8
- Allen, P. G.; Conradson, S. D.; Wilson, M. S.; Gottesfeld, S.; Raistrick, I. D.; Valerio, J.; Lovato, M. 1994. In-situ Structural Characterization of a Platinum Electrocatalyst by Dispersive X-ray Absorption Spectroscopy, *Electrochim. Acta* (39) 2415-2418
- Tyson, T. A.; Conradson, S. D.; Farrow, R. F. C.; Jones, B. A. 1996. Observation of Internal Interfaces in $\text{Pt}_x\text{Co}_{1-x}$ ($x \sim 0.7$) Alloy Films: A Likely Cause of Perpendicular Magnetic Anisotropy, *Phys. Rev. B* (54) R3702-R370
- Tyson, T. A.; de Leon, J. M.; Conradson, S. D.; Bishop, A. R.; Neumeier, J. J.; Roder, H.; Zang, J. 1996. Evidence for a Local Lattice Distortion in Ca-Doped LaMnO_3 , *Phys. Rev. B* (53) 13985-13988
- Ankudinov, A.L.; Ravel, B.; Rehr, J. J.; Conradson, S. D. 1998. Real-Space Multiple-Scattering Calculation and Interpretation of X-ray Absorption Near Edge Structure, *Phys. Rev. B* (58) 7565-76
- Conradson, S. D. et al. 2005. Local and Nanoscale Structure and Speciation in the $\text{PuO}_{2+x-y}(\text{OH})_2\text{H}_2\text{O}$ System, *J. Am. Chem. Soc.* (126) 13443-13458.
- Conradson, S. D. et al. 2005. Charge Distribution and Local Structure and Speciation in the UO_{2+x} and PuO_{2+x} Binary Oxides for $x \leq 0.25$, *J. Solid State Chem.* (178) 521-535.
- Garcia-Adeva, A. J., Howell, R. C., Conradson, S. D., de Leon, J. M., Espinosa-Faller, F. J. 2005. Local Atomic Structure of Partially Ordered NiMn in NiMn/NiFe Exchange-Coupled Layers: II. Electronic Structure Calculations, *J. Phys. Chem. B*, (109) 10419-10428.

COLLABORATORS

David Clark (LANL), Piotr Zelenay (LANL), Alan Bishop (LANL), Hans Frauenfelder (LANL), Nancy Hess (PNL), Christophe den Auwer (CEA Marcoule), Carole Valot (CEA Cadarache), Eric Simoni (University Sud Paris, Orsay), Takeshi Egami (UTK), Gerry Lander (ITU), Dragan Mihailovic (JSI Ljubljana), Davor Pavuna (EPFL), Ivan Bozovic (BNL), Stuart Parking (IBM Almaden)

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EDUCATION

1977 Ph.D. Environmental Engineering and Sciences, Stanford University. Adviser, James Leckie.
1972 B.S. Chemical Engineering, Carnegie-Mellon University, Pittsburgh, PA.

PROFESSIONAL EXPERIENCE

1980-2008: U.S. Geological Survey, Water Resources Division, Menlo Park, CA.
1989-1990: Visiting Scientist, Australian Nuclear Science and Technology Organization, Lucas Heights, Australia.

James A. Davis is a Senior Research Hydrologist at the U. S. Geological Survey (Menlo Park, CA), whose research focuses on geochemical processes occurring at mineral surfaces and their effects on water quality in natural water systems. The research includes: a) Field investigations of contaminant transport at various physical scales and in differing geochemical regimes, including current studies of how transport of uranium in aquifers is affected by adsorption, redox reactions, and competitive sorption processes, b) Reactive transport modeling under conditions that apply to various environmental settings, including transport coupled with adsorption, and c) Laboratory studies of sorption and transport of inorganic ions and description of the results with geochemical models that include surface complexation. A simple approach to modeling the influence of variable chemistry on metal ion adsorption and transport has been demonstrated at two field sites at the km scale (Naturita, CO and Cape Cod, MA). These studies constitute a major advance in applying the surface complexation concept to natural systems.

AWARDS

Noted as author of one of the 10 most cited articles in journal history, *Environmental. Sci. Tech.*, 2001.
Distinguished Service Award, Dept. of Interior, for outstanding scientific contributions, 2000.

PROFESSIONAL AFFILIATIONS

American Chemical Society
American Geophysical Union
Geological Society of America
Geochemical Society

RELEVANT PROFESSIONAL ACTIVITIES

- Organizing Committee, DOE Workshop on Basic Research Needs for the Geosciences, Nuclear Waste Disposal and Carbon Sequestration, 2006-2007.
- Co-Chairman, Working Group on Subsurface Reactive Transport Modeling, Interagency Steering Committee on Multimedia Environmental Models, 2003-2006.
- Technical Direction Team, Sorption Project, Nuclear Energy Agency (OECD, Paris): 2002-2006.
- Program Committee, Geotrap-V Workshop on the Transport of Radionuclides in Heterogeneous Geologic Media: May 2001.
- Invited Speaker, Gordon Conference, Nuclear Waste and Energy: July 2000.
- Associate Editor, Water Resources Research: 1997-2001.
- Symposium Co-Chairman for "Groundwater Remediation of Trace Metals, Radionuclides, and Nutrients with Permeable Reactive Barriers", AGU National Meeting, San Francisco: 1999.

- Executive Committee, Hydrology Section, American Geophysical Union: 1995-1997.
- Chairman, Geochemistry Division, American Chemical Society: 1991-1992

PUBLICATIONS (10 Recent relevant publications)

- Arai, Y., Marcus, M.A., Tamura, N., Davis, J.A., and Zachara, J.M. 2007. Spectroscopic evidence for uranium bearing precipitates in vadose zone sediments at the Hanford 300-area site. *Environmental Science and Technology*, 41, 4633-4639.
- Curtis, G. P., J. A. Davis, and D. L. Naftz. 2006. Simulation of reactive transport of uranium(VI) in groundwater with variable chemical conditions. *Water Resources Research* 42, W044404, doi:10.1029/2005WR003979.
- Arai, Y., McBeath, M., Bargar, J.R., Joye, J., and Davis, J.A. 2006. Uranyl adsorption and surface speciation at the imogolite-water interface: Self-consistent spectroscopic and surface complexation models. *Geochimica et Cosmochimica Acta*, 70, 2492-2509.
- Davis, J.A., Curtis, G.P., Wilkins, M.J., Kohler, M., Fox, P.M., Naftz, D.L., and Lloyd, J.R. 2006. Processes affecting transport of uranium in a suboxic aquifer. *Physics and Chemistry of the Earth*, 31, 548-555.
- Fox, P.M., Davis, J.A., and Zachara, J.M. 2006. The effect of calcium on aqueous uranium (VI) speciation and adsorption to ferrihydrite and quartz. *Geochimica et Cosmochimica Acta*, 70, 1379-1387.
- Davis, J.A., Yabusaki, S.B., Steefel, C.I., Zachara, J.M., Curtis, G.P., Redden, G.D., Criscenti, L.J., and Honeyman, B.D. 2004. Assessing conceptual models for subsurface reactive transport of inorganic contaminants. *EOS*, 85, 449-455.
- Curtis, G.P., Fox, P., Kohler, M., and Davis, J. A. 2004. Comparison of field uranium K_d values with a laboratory determined surface complexation model. *Applied Geochemistry*, 19, 1643-1653.
- Payne, T.E., Davis, J.A., Ochs, M., Olin, M. and Tweed, C.J. 2004. Uranium adsorption on weathered schist – Intercomparison of modeling approaches. *Radiochimica Acta*, 92, 651-661.
- Davis, J.A., Meece, D.M., Kohler, M., and Curtis, G. P. 2004. Approaches to surface complexation modeling of uranium(VI) adsorption on aquifer sediments. *Geochimica et Cosmochimica Acta*, 68, 3621-3641.
- Barger, J.R., Reitmeyer, R, Lenhart, J.J., and Davis, J.A. 2000. Characterization of U(VI)-carbonato ternary complexes on hematite: EXAFS and electrophoretic mobility measurements. *Geochimica et Cosmochimica Acta*, 64, 2737-2749.

COLLABORATORS

Y. Arai (Clemson), J. R. Bargar (SSRL), K. Hayes (Univ. of Michigan), B. Honeyman (Colorado School of Mines), C. Steefel (LBNL), P. Long (PNNL), G. Waychunas (LBNL), J. Zachara (PNNL).

SCOTT FENDORF

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EDUCATION

1988 B.S. in Soil Science; California Polytechnic State University, SLO

1990 M.S. in Soil Chemistry; University of California, Davis

1992 Ph.D. Soil/Environ. Chemistry; University of Delaware

EXPERIENCE

Professor Fendorf's research seeks to define the chemical processes (including biologically mediated chemical processes) that drive the cycling and fate of trace elements within soils, sediments, and groundwater. His efforts focus on reactions influencing the partitioning of elements between soil solutions and solids—particularly redox processes at the solid-water and microbe-mineral interfaces. His studies span the spatial range from microscopic examination of trace element partitioning on soil minerals to field-scale observations of seasonal cycling pathways. Using a host of spectroscopic and microscopic techniques, Professor Fendorf has sought to quantify temporal and micro-scale spatial variation in biogeochemical processes within soils and sediments. He has been a pioneer of synchrotron X-ray techniques to the study of soil processes and is currently using spectroscopic, scattering, and tomographic means to identify metal transformations within the physical complexity of soils and sediments.

PROFESSIONAL AFFILIATIONS

- Member of the American Geophysical Union
- Member of the American Society of Agronomy.
- Member of the Soil Science Society of America.
- Member of the American Chemical Society.
- Member of the Geochemical Society

RELEVANT PROFESSIONAL ACTIVITIES

Symposium Organizer, “Arsenic Dynamics within Soils and Sediments”, Soil Science Society of America National Meeting, Denver, 2003.

Symposium Organizer, “Mechanisms of Electron Transfer at the Mineral-Water Interface”, Soil Science Society of America National Meeting, Seattle, 2004.

Organizing Committee for 2005 Geochemical Society's Goldschmidt Conference, Moscow, ID.

Organizing Committee for 2005 ISSM-ISEB Symposia, Jackson Hole, WY.

Participant in National Science Foundation Workshop on “Frontiers in Exploration of the Critical Zone”, 2005.

Participant and speaker for National Academy of Science's workshop on “Frontiers in Soil Science Research”, 2005.

Guest Editor, *Chemical Geology* special issue on “Controls on Arsenic Transport in Near-Surface Aquatic Systems”. 2006.

Facility Representative for the Environmental Spectroscopy and Biogeochemistry Program, and member of the Advisory Council, Environmental Molecular Science Laboratory, Pacific Northwest National Laboratory. 2007-.

Associate Editor, *Vadose Zone Journal*. 2008-

SELECTED RECENT PUBLICATIONS (>100 total refereed publications)

- Hansel, C. M., S. Fendorf, P. M. Jardine, C. A. Francis. 2008. Changes in bacterial and archaeal community structure and functional diversity along a geochemically variable soil profile. *Appl. Environ. Microbiol.* In press.
- Bank, T.L., T.A. Vishnivetskaya, P.M. Jardine, M. Ginder-Vogel, S. Fendorf, M.E. Baldwin. 2007. Elucidating geochemical and biogeochemical uranium reduction on neutral, reducing soils. *Geomicrobiology Journal* 24:125-132.
- Borch, T., Y. Masue, R. K., Kukkadapu, and S. Fendorf. 2007. Phosphate imposed limitations in biological reduction and alteration of ferrihydrite. *Environ. Sci. Technol.* 41: 166-172.
- Neiss, J., B. Stewart, P. Nico, S. Fendorf. 2007. Geochemical constraints on microbially mediated uranyl reduction. *Environ. Sci. Technol.* 41: 7343-7348.
- Oze, C., D.K. Bird, and S. Fendorf. 2007. Genesis of hexavalent chromium from natural sources in soil and groundwater. *PNAS* 104: 6544-6549
- Stewart, B. D., J. Neiss, and S. Fendorf. 2007. Quantifying constraints imposed by calcium and iron on bacterial reduction of uranium(VI). *J. Environ. Qual.* 36: 363-372.
- Ginder-Vogel, M. A., C. Criddle, and S. Fendorf. 2006. Thermodynamic constraints on the oxidation of biogenic UO₂ by Fe(III) (hydr)oxides. *Environ. Sci. Technol.* 40: 3544-3550.
- Ginder – Vogel, M., T. Borch, M. Mayes, P. Jardine, and S. Fendorf. 2005. Chromate reduction and retention processes within Hanford sediments. *Environ. Sci. Technol.* 39: 7833-7839.
- Hansel, C.M., S. G. Benner, S. Fendorf. 2005. Competing Fe(II)-induced mineralization pathways of ferrihydrite. *Environ. Sci. Technol.* 39: 7147-7153.
- Hansel, C.M., S. Benner, P.S. Nico, and S. Fendorf. 2004. Structural constraints of ferric (hydr)oxides on dissimilatory iron reduction and the fate of Fe(II). *Geochim. Cosmochim. Acta* 68: 3217-3229.
- Brooks, S.C., J. K. Fredrickson, S. L. Carroll, D.W. Kennedy, J. M. Zachara, A. E. Plymale, S. D. Kelley, K. M. Kemner, and S. Fendorf. 2003. Inhibition of U(VI) reduction by Ca. *Environ. Sci. Technol.* 37: 1850-1858.
- Hansel, C.M., S. Benner, Dohnalkova, A., R.K. Kukkadapu, and S. Fendorf. 2003. Secondary mineralization pathways induced by dissimilatory iron reduction of ferrihydrite under advective flow. *Geochim. Cosmochim. Acta* 67: 2977-2992.
- Benner, S.G., C.H. Hansel., B.W. Wielinga, T.M. Barber, and S. Fendorf. 2002. Reductive dissolution and biomineralization of iron hydroxide under dynamic flow conditions. *Environ. Sci. Technol.* 36: 1705-1711.
- Fendorf, S., B.W. Wielinga, and C.M. Hansel. 2002. Operative pathways of chromate and uranyl reduction within soils and subsurface media. In P.C. Zhang and P. Brady (Eds.) *Soil Geochemical Processes of Radionuclides*. Soil Sci. Soc. Am. Special Publication. P. 111-130.
- Fendorf, S., B.W. Wielinga, and C.M. Hansel. 2000. Chromium transformations in natural environments: The role of biological and abiological processes in chromium(VI) reduction. *Internat. Geol. Rev.* 42:691-701.
- Wielinga, B., B. Bostick, R.F. Rosenzweig, and S. Fendorf. 2000. Inhibition of bacterially promoted uranium reduction: Ferric (hydr)oxides as competitive electron acceptors. *Environ. Sci. Technol.* 34:2190-2195.

COLLABORATORS

Dr. Mark Barnett (Auburn); Dr. S.G. Benner (BSU); Dr. C. F. Harvey (MIT); Dr. P.M. Jardine (ORNL); Dr. W. Inskeep (Montana State University); Dr. Ravi Kukkadapu; Dr. Melanie Mayes (ORNL); Dr. M.J. Morra (University of Idaho); Dr. J. Zachara (PNNL)

KEN KEMNER

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EDUCATION

Naval Research Laboratory, National Research Council Postdoctoral Fellow, 1993-1996
University of Notre Dame, Ph.D., 1993, Physics
Xavier University, B.S., 1986, Physics

EXPERIENCE

Dr. Kemner has performed extensive experimental research in Materials Science and Molecular Environmental Science via the development and application of synchrotron-based methods. Since 1996, when he began work at Argonne National Laboratory, he has been developing the Molecular Environmental Science Research Group, an integrated multidisciplinary research group consisting of physicists, chemists, and microbiologists who are interested in making use of third generation synchrotron radiation for environmental research. Since 1997, he has been investigating mineral-microbe-metal interactions and their role in effecting the transformations of contaminant metals and radionuclides. The research has ranged from studies of laboratory-derived samples to field samples. Dr. Kemner's current research is focused on understanding coupled microbiological and geochemical processes, particularly at the mineral-microbe interface, and their effect on the transformations of contaminant metals and radionuclides. In addition to making extensive use of x-ray absorption fine structure spectroscopy, he also leads the development of nanospectroscopy approaches to investigate the mineral-microbe interface.

PROFESSIONAL AFFILIATIONS

- American Chemical Society
- American Physical Society
- American Society of Microbiology
- American Association for the Advancement of Science
- American Geophysical Union
- Mineralogical Society of America
- International XAFS Society

RELEVANT PROFESSIONAL ACTIVITIES

- Co-creator of Synchrotron Environmental Science (SES) Series Conference; Co-organizer of SES-I and SES-II (1999 and 2002)
- International Scientific Committee for 3rd and 4th Workshops on Speciation, Techniques, and Facilities for Radioactive Materials at Synchrotron Light Sources, 2003-2006.
- Executive Committee Member of MRCAT/EnviroCAT (1996-present)
- University of Notre Dame Center for Environmental Science and Technology Advisory Board, 2003-2007.

SELECTED PUBLICATIONS (from over 90)

S. D. Kelly, K. M. Kemner, J. Carley, C. Criddle, P. M. Jardine, T. L. Marsh, D. Phillips, D. Watson, W. Wu, "Speciation of Uranium in Sediments before and after in Situ Biostimulation," *Environ. Science and Technol.* (accepted)

M. J. Daly, E. K. Gaidamakova, V. Y. Matrosova, A. Vasilenko, M. Zhai, K. M. Kemner, B. Lai, B.

- Ravel, L. P. Wackett, S. W. Li, J. K. Fredrickson, "Protein Oxidation Implicated as the Primary Determinant of Bacterial Radioresistance," *PLoS Biology* Vol. 5, No. 4, e92
doi:10.1371/journal.pbio.0050092.
- M. J. Marshall, A. Beliaev, A. C. Dohnalkova, D. Kennedy, L. Shi, Z. Wang, M. Boyanov, B. Lai, K. M. Kemner, J. S. McLean, S. B. Reed, D. E. Culley, V. L. Bailey, C. J. Simonson, D. A. Saffarini, M. F. Romine, Y. Gorby, J. M. Zachara, J. K. Fredrickson, "c-Type Cytochrome-Dependent Formation of U(IV) Nanoparticles by *Shewanella oneidensis*," *PLoS Biology*, Vol. 4, Issue 8.
- K. M. Kemner, S. D. Kelly, "Synchrotron-based Techniques for Monitoring Metal Transformations," *Manual of Environmental Microbiology Third Edition (2007)*, Editor in chief: Christon J. Hurst, ASM Press 1183-1194.
- K. M. Kemner, E. J. O'Loughlin, S. D. Kelly, M. I. Boyanov, "Synchrotron x-ray investigations of mineral-microbe-metal interactions," *Elements* August, 2005, pg. 217-221.
- K. M. Kemner, E. J. O'Loughlin, S. D. Kelly, B. Ravel, M. Boyanov, D. Sholto-Douglas, B. Lai, R. Cook, E. Carpenter, V. Harris, K. H. Nealson, "XAFS and X-ray and Electron Microscopy Investigations of Radionuclide Transformations at the Mineral-Microbe Interface" *American Institute of Physics*, 882 250-252, 2007.
- K. M. Kemner, S. D. Kelly, B. Lai, J. Maser, E. J. O'Loughlin, D. Sholto-Douglas, Z. Cai, M. A. Schneegurt, C. F. Kulpa, Jr., K. H. Nealson, "Elemental and Redox Analysis of Single Bacterial Cells by X-ray Microbeam Analysis," *SCIENCE*, 306 686-687, 2004.
- E. J. O'Loughlin, S.D. Kelly, R.E. Cook, R. Csencsits, and K.M. Kemner, "Reduction of uranium(VI) by mixed Fe(II)/Fe(III) hydroxide (green rust): Formation of UO₂ nanoparticles," *Environ. Sci. Technol.* 37 721-727, 2003.
- S. C. Brooks, J. K. Fredrickson, S. L. Carroll, D. W. Kennedy, J. M. Zachara, A. E. Plymale, S. D. Kelly, K. M. Kemner, and S. Fendorf, "Inhibition of Bacterial U(VI) reduction by calcium," *Environ. Sci. Technol.* 37 1850-1858, 2003.
- S. D. Kelly, K. M. Kemner, J. B. Fein, D. A. Fowle, M. I. Boyanov, B. A. Bunker, N. Yee, "X-ray absorption fine structure determination of pH-dependent U-bacterial cell wall interactions," *Geochimica et Cosmochimica Acta.*, 66 3855-3871, 2002.
- S. Kelly, M. Newville, L. Cheng, K. M. Kemner, S. Sutton, P. Fenter, N. Sturchio, C. Spotl, "Uranyl incorporation in natural calcite," *ES&T* 37 1284-1287, 2003.
- Y. Suzuki, S. D. Kelly, K. M. Kemner, J. F. Banfield, "Nanometer-size products of uranium bioreduction," *Nature* 419 134, 2002.
- M. I. Boyanov, E. J. O'Loughlin, E. E. Roden, J. B. Fein, K. M. Kemner, "Adsorption of Fe(II) and U(VI) to carboxyl-functionalized microspheres: the influence of speciation on uranyl reduction studies by titration and XAFS," *Geochim. Cosmochim. Acta* 71 1898-1912, 2007.
- M. Labrenz, G. K. Druschel, T. Thomsen-Ebert, B. Gilbert, S. A. Welch, K. M. Kemner, G. A. Logan, R. E. Summons, G. De Stasio, P. L. Bond, B. Lai, S. D. Kelly, J. F. Banfield, "Sphalerite (ZnS) deposits forming in natural biofilms of sulfate reducing bacteria," *Science* 290 1744-1747, 2000.
- K. M. Kemner, B. Lai, J. Maser, M. A. Schneegurt, Z. Cai, P. P. Ilinski, C. F. Kulpa, D. G. Legnini, K. H. Nealson, S. T. Pratt, W. Rodrigues, M. Lee Tischler, W. Yun, "Use of The High-energy X-ray Microprobe At The Advanced Photon Source To Investigate The Interactions Between Metals And Bacteria," *X-Ray Microscopy: Proceedings of the Sixth International Conference*, pg. 319-322, 2000, American Institute of Physics.

COLLABORATORS

Scott Brooks (ORNL); Jim Fredrickson (PNNL); John Zachara (PNNL); Michelle Scherer (University of Iowa); Bill Burgos (Pennsylvania State University); Jeremy Fein (University of Notre Dame)

ROB KNIGHT

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EDUCATION

1996 BS University of Otago, Biochemistry

2001 Ph.D. Princeton University, Ecology and Evolutionary Biology

2001-2004 Postdoc University of Colorado, Molecular, Cellular and Developmental Biology

ACADEMIC/PROFESSIONAL APPOINTMENTS

Assistant Professor, Chemistry and Biochemistry, University of Colorado, 8/04 – present

FIVE MOST RELEVANT PUBLICATIONS (*Out of 54 Total*)

Lozupone, C., Hamady, M. and Knight, R. (2006) “UniFrac: An Online Tool for Comparing Microbial Community Diversity in a Phylogenetic Context”. *BMC Bioinformatics* 7:371.

Lozupone, C.A., and Knight, R. (2007) “Global patterns in bacterial diversity”. *PNAS* 104:11436-40.

Turnbaugh, P.J., Hamady, M., Ley, R., Fraser, C., Knight, R., and Gordon, J.I. (2007) “The human microbiome project: exploring the microbial side of ourselves”. *Nature* 449:804.

Ley, R.E., Backhed, F., Turnbaugh, P., Lozupone, C.A., Knight, R.D., and Gordon, J.I. "Obesity alters gut microbial ecology." (2005). *Proceedings of the National Academy of Sciences*. 102:11070-11075.

Knight, R., Maxwell, P., Birmingham, A., Carnes, J., Caporaso, J.G., Easton, B.C., Hamady, M., Liu, Z., Lozupone, C., Sammut, R., Smit, S., Wakefield, M., Widmann, J., Wikman, S., Wilson, S., and Huttley, G.A.. (2007) “PyCogent: a toolkit for making sense from sequence”. *Genome Biology* 8:R171.

FIVE OTHER SIGNIFICANT PUBLICATIONS

Knight, R., De Sterck, H., Markel, R., Smit, S., Oshmyansky, A., and Yarus, M. (2005) "Abundance of correctly folded RNA motifs in sequence space, calculated on computational grids". *Nucleic Acids Research* 33:5924-35.

Hamady, M., Walker, J.J., Harris, J.K., Gold, N., and Knight, R. “Error-correcting barcoded primers allow hundreds of samples to be pyrosequenced in multiplex”. In press, *Nature Methods*.

Knight, R. D. and L. F. Landweber (2000). "The Early Evolution of the Genetic Code" *Cell* 101(6): 569-572.

Xu, J., Mahowald, M.A., Ley, R.E., Lozupone, C.A., Hamady, M., Martens, E.C., Henrissat, B., Coutinho, P.M., Minx, P., Latreille, P., Cordum, H., Van Brunt, A., Kim, K., Fulton, R.S., Fulton, L.A., Clifton, S.W., Wilson, R.K., Knight, R.D., Gordon, J.I. (2007). “Evolution of symbiotic bacteria in the distal human intestine”. *PLoS Biology* 5:e156.

Freeland, S. J., R. D. Knight, and L. F. Landweber (1999). "Do proteins predate DNA?" *Science* 286(5440): 690-2.

SYNERGISTIC ACTIVITIES

Faculty member, University of Colorado Health Sciences Center Computational Bioscience Program, 2004-pres., and CU Boulder Department of Computer Science, 2006-pres.

Organizer, Bioinformatics Supergroup, CU Boulder, 2002-pres. I initiated this multidisciplinary research seminar as a postdoc, and continue to run it.

Recruitment and research training of undergraduate students through SMART (Summer Multicultural Access to Research Training), UROP (Undergraduate Research Opportunities Program), and URAP (Undergraduate Research Assistantship Program).

Session co-organizer, “The Modern RNA World”, Evolution meeting 2005, Auckland, New Zealand, June 19-23.

Member, RNA Ontology Consortium, 2006-pres.

OTHER COLLABORATORS

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EDUCATION

1986 B.S. University of Hohenheim, Germany, Biology, Agricultural Sciences

1990 M.S. University of Hohenheim, Germany; Microbiology, Biochemistry

1994 Ph.D. Technical Univ. Harburg/Hohenheim, Technical Biochemistry/Microbiology

1994-1999 Postdoc Michigan State University, Microbiol Ecology

EXPERIENCE

4/2004-Present	Associate Professor	Environmental Engineering, Georgia Tech
1/2003	Adjunct Professor	School of Biology, Georgia Tech
4/1999-Present	Assistant Professor	Environmental Engineering, Georgia Tech
1997-1999	Research Associate	Michigan State University
1994-1996	Feodor-Lynen Fellow	Michigan State University
1990-1994	Graduate Research Assistant	Technical University Hamburg-Harburg
1986-1990	Undergraduate Research Assistant	University of Hohenheim, Stuttgart

PUBLICATIONS

- Sanford RA, Wu Q, Sung Y, Thomas SH, Amos BK, Prince EK, Löffler FE. 2007. Hexavalent uranium supports growth of *Anaeromyxobacter dehalogenans* and *Geobacter* spp. with lower than predicted biomass yields. *Environ. Microbiol.* 9:2885-2893.
- Bedard DL, Ritalahti KM, Löffler FE. 2007. The *Dehalococcoides* population in sediment-free mixed cultures metabolically dechlorinates the commercial polychlorinated biphenyl mixture aroclor 1260. *Appl. Environ. Microbiol.* 73:2513-2521.
- Wu Q, Sanford RA, Löffler FE. 2006. Uranium(VI) reduction by *Anaeromyxobacter dehalogenans* strain 2CP-C. *Appl. Environ. Microbiol.* 72:3608-3614.
- Krajmalnik-Brown, R., T. Hölscher, I. N. Thomson, F. M. Saunders, K. M. Ritalahti, and F. E. Löffler. 2004. Genetic identification of a putative vinyl chloride reductase in *Dehalococcoides* sp. strain BAV1. *Appl. Environ. Microbiol.* 70:6347-6351.
- Ritalahti, K. M., and F. E. Löffler. 2004. Populations implicated in the anaerobic reductive dechlorination of 1,2-dichloropropane in highly enriched bacterial communities. *Appl. Environ. Microbiol.* 70:4088-4095.
- He, J., K. M. Ritalahti, K.-L. Yang, S. S. Koenigsberg, and F. E. Löffler. 2003. Detoxification of vinyl chloride to ethene coupled to growth of an anaerobic bacterium. *Nature* 424:62-65.
- He, J., K. M. Ritalahti, M. R. Aiello, and F. E. Löffler. 2003. Complete detoxification of vinyl chloride by an anaerobic enrichment culture and identification of the reductively dechlorinating population as a *Dehalococcoides* species. *Appl. Environ. Microbiol.* 69:996-1003.
- Griffin, B. M., J. M. Tiedje, and F. E. Löffler. 2004. Anaerobic microbial reductive dechlorination of tetrachloroethene to predominately *trans*-1,2-dichloroethene. *Environ. Sci. Technol.* 38:4300-4303.
- Sung, Y, K.M. Ritalahti, R.A. Sanford, J.W. Urbance, S.J. Flynn, J.M. Tiedje, and F.E. Löffler. 2003. Characterization of two tetrachloroethene-reducing, acetate-oxidizing anaerobic bacteria, and their description as *Desulfuromonas michiganensis* sp. nov. *Appl. Environ. Microbiol.* 69:2964-2974.

He, J. Y. Sung, M. E. Dollhopf, B. Z. Fathepure, J. M. Tiedje, and F. E. Löffler. 2002. Acetate versus hydrogen as direct electron donors to stimulate the microbial reductive dechlorination process at chloroethene-contaminated sites. *Environ. Sci. & Technol.* 36:3945-3952.

Löffler, F. E., Q. Sun, J. Li, and J. M. Tiedje. 2000. 16S rRNA gene-based detection of tetrachloroethene (PCE)-dechlorinating *Desulfuromonas* and *Dehalococcoides* species. *Appl. Environ. Microbiol.* 66:1369-1374.

Löffler, F. E., J. M. Tiedje, and R. A. Sanford. 1999. The fraction of electrons consumed in electron acceptor reduction (f_e) and hydrogen thresholds as indicators of halorespiratory physiology. *Appl. Environ. Microbiol.* 65:4049-4056.

COLLABORATORS & OTHER AFFILIATIONS

Abriola, L.	Univ. of Michigan	Hunt, W.	Georgia Tech	Ramsburg, A.	Tufts University
Adriaens, P.	Univ. of Michigan	Koenigsberg, S.	Regenesis	Ritalahti, K.	Georgia Tech
Adrian, L.	Technical Univ. Berlin	Lendvay, J.	Univ. of San Francisco	Sanford, R.	Univ. of Illinois
Cole, J.	Michigan State Univ.	Pennell, K.	Georgia Tech	Sobecky, P.	Georgia Tech
Fathepure, B.	Oklahoma State Univ.	Petrovskis, E.	GeoSyntec Consultants	DiChristina, T.	Georgia Tech.

MELANIE A. MAYES

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EDUCATION

University of Tennessee, Ph.D., 2006, Geological Sciences
University of Tennessee, M.S., 1999, Geological Sciences
University of Missouri, B.S., 1995, Geological Sciences

EXPERIENCE

Dr. Mayes conducts experimental and theoretical research on the coupled hydrological and geochemical transport of metals, chelated metals, radionuclides, and natural constituents in soil and ground waters. Her specialty is in designing innovative collection strategies and experiments to interrogate pore-scale mechanisms of water and contaminant exchange in field-relevant, intact sediments. She currently serves as principal investigator on an ERSP-funded investigation using laboratory-scale, layered Hanford sediments collected from over a range of spatial scales (0.02 – 1 m). She also leads a combined experimental and modeling investigation using intact layered sediments (0.2m) from a variety of sedimentary facies on the Hanford site supported by the Tank Farm Vadose Zone Project.

PROFESSIONAL AFFILIATIONS

- American Chemical Society
- American Geophysical Union
- Soil Science Society of America
- National Ground Water Association

RELEVANT PROFESSIONAL ACTIVITIES

- Associate Editor, Soil Science Society of America Journal

SELECTED PUBLICATIONS

- Pace, M.N., Mayes, M.A., Jardine, P.M., McKay, L.D., Yin, X.L., Mehlhorn, T.L., Liu, Q., and H. Gürleyük. 2007. Transport of Sr^{2+} and SrEDTA^{2-} in partially-saturated and heterogeneous sediments. *J. Contam. Hydrol.* 91:267-287.
- Gwo, J.-P., Mayes, M.A., and Jardine, P.M. 2007. Quantifying the physical and chemical mass transfer processes for the fate and transport of Co(II)EDTA in a partially-weathered limestone-shale saprolite. *J. Contam. Hydrol.* 90:184-202.
- Jardine, P.M., Mayes, M.A., Mulholland, P.J., Hanson, P.J., Tarver, J.R., Luxmoore, R.J., McCarthy, J.F., and Wilson, G.V. 2006. Vadose zone flow and transport of dissolved organic carbon at multiple scales in humid regimes. *Vadose Zone J.* 5:140-152.
- Ginder-Vogel, M., Borch, T., Mayes, M.A., Jardine, P.M., and Fendorf, S.E. 2005. Chromate reduction and retention processes within Hanford sediments. *Environ. Sci. Technol.* 39:7833-7839.
- Mayes, M.A., Mehlhorn, T.L., and Jardine, P.M. 2005. Coupled hydrological and geochemical processes influencing the transport of chelated metals in the ORNL vadose zone and groundwater. ACS Symposium Series 910: Biogeochemistry of Chelating Agents, Nowack, B. and Van Briesen, J., Eds., pp. 297-315.

- Mayes, M.A., Yin, X.L., Pace, M.N., and Jardine, P.M. 2005. Rates and mechanisms of Co(II)EDTA²⁻ interactions with sediments from the Hanford site. In: ACS Symposium Series 910: Biogeochemistry of Chelating Agents, Nowack, B. and Van Briesen, J., Eds., pp. 278-296.
- Mayes, M.A., Pace, M. N., Jardine, P.M., Fendorf, S.E., Farrow, N.D., Yin, X.L., and Zachara, J.M. 2005. Coupled hydrological and geochemical processes governing the fate and transport of Sr and U in the Hanford vadose zone. ACS Symposium Series 904: Subsurface Contamination Remediation: Accomplishments of the Environmental Management Science Program, Zachry, T., and Berkey, E., Eds., pp. 229-250.
- Mayes, M.A., Jardine, P.M., Mehlhorn, T.L., Bjornstad, B.N., Ladd, J.L., and Zachara, J.M. 2003. Transport of multiple tracers in variably saturated humid region structured soils and semi-arid region laminated sediments. *J. Hydrol.* 275: 141-161.
- Pace, M.N., Mayes, M.A., Jardine, P.M., Mehlhorn, T.L., Zachara, J.M., and Bjornstad, B.N. 2003. Quantifying the effects of small-scale heterogeneities on flow and transport in undisturbed cores from the Hanford Formation. *Vadose Zone J.* 2: 664-676.
- Gwo, J.P., D'Azevedo, E.F., Frenzel, H., Mayes, M.A., Yeh, G.-T., Jardine, P.M., Salvage, K.M., and Hoffman, F.M. 2001. HBGC123D: a high performance computer model of coupled hydrological and biogeochemical processes. *Computer and Geosciences* 27: 1231-1242.
- Mayes, M.A., Jardine, P.M., Larsen, I.L., Brooks, S.C., and Fendorf, S.E. 2000. Multispecies transport of metal-EDTA and chromate complexes through undisturbed columns of weathered fractured saprolite. *J. Contam. Hydrol.* 45: 243-265.
- Jardine, P.M., Fendorf, S.E., Mayes, M. A., Larsen, I.L., Brooks, S.C., and Bailey, W.B. 1999. Fate and transport of hexavalent chromium in undisturbed heterogeneous soil. *Environ. Sci. Technol.* 33: 2939-2944.

COLLABORATORS

Phil Jardine (ORNL), Ed Perfect (University of Tennessee), Jack Parker (University of Tennessee), Scott Fendorf (Stanford University), Scott Brooks (ORNL)

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EDUCATION

University of Birmingham, UK, 1988, PhD Biochemistry
University of Keele, UK, 1985, BSc Biochemistry

EXPERIENCE

Professor Richardson has a long established track record for biochemical studies on bacterial respiratory systems, most notably those of the nitrogen and iron cycles. His group has produced structure-function descriptions of nitrate, nitrite reductases and multi-heme c-type cytochromes involved in electron transfer to these enzymes. He has also produced detailed spectropotentiometric characterisation of the MtrA and MtrC decaheme proteins involved in Fe(III) respiration by *Shewanella* species. He is director of the Centre for Metalloprotein Spectroscopy and Biology that is a multidisciplinary biophysical chemistry group with expertise in a range of methodologies for protein structure and function studies that include X-ray crystallography, NMR spectroscopy, analytical ultracentrifugation, electron paramagnetic spectroscopy, magnetic circular dichroism and protein film voltammetry.

AWARDS and HONOURS

Royal Society Wolfson Merit Award Holder (2007-2012)
Fleming Medal Lecturer 1999

PROFESSIONAL AFFILIATIONS

- Biochemical Society
- Society for General Microbiology
- American Society for Biochemistry and Molecular Biology

RELEVANT PROFESSIONAL ACTIVITIES

Director, Centre for Metalloprotein Spectroscopy and Biology
Honorary Editor, Biochemical Society Transactions
Editorial Board Member, 'Journal of Biological Chemistry' 2003-2007
Associate Editor 'Microbiology' 2000-2005
Vice-Chair European Commission COST Action 856 on 'Denitrification'
Member, Faculty 1000 e-review group
Member, Aurora Advisory Committee on space missions to Mars

RELEVANT RECENT PUBLICATIONS (*from ~160*)

- Hartshorne RS, Jepson B, Clarke, TC, Field SJ, Fredrickson J, Zachara J, Shi L, Butt JN, Richardson DJ (2007) Characterisation of *shewanella oneidensis* MtrC: a cell surface decaheme cytochrome involved in respiratory electron transport of extracellular electron acceptors. *J. Biol. Inorg. Chem.* 12:1083-1094
- Clarke TA, Cole JA, Richardson DJ, Hemmings AM. (2007) The crystal structure of the pentahaem c-type cytochrome NrfB and characterisation of its solution-state interaction with the pentahaem nitrite reductase NrfA. *Biochem J.* 4-6:19-30
- Jepson B, Mohan S, Clarke T, Gates AJ, Cole JA, Butt JN, Hemmings AM, Richardson DJ (2007) Spectropotentiometric and structural characterisation of the periplasmic nitrate reductases of *Escherichia coli*. *J. Biol. Chem.* 282:6425-37.

- Hartshorne RS, Kern M, Meyer B, Clarke TA, Richardson DJ, Simon S (2007) Unconventional covalent heme binding in a novel bacterial cytochrome *c* requires a dedicated heme lyase. *Mol. Microbiol.* 64:1049-60
- Thorndycroft FH, Butland G, Richardson DJ, Watmough NJ. (2007) A new assay for nitric oxide reductase reveals two conserved glutamate residues form the entrance to a proton-conducting channel in the bacterial enzyme. *Biochem J.* 401:111-119.
- Southall S, Joel J, Richardson DJ, Oubrie A (2006). Structural and kinetic characterisation of a novel aldose sugar dehydrogenase from *Escherichia coli* (2006) *J. Biol. Chem.* 281, 30650-30659
- Gwyer JD, Richardson DJ, Butt JN. (2005) Diode or tunnel-diode characteristics? Resolving the catalytic consequences of proton coupled electron transfer in a multi-centered oxidoreductase. *J Am Chem Soc.* 2005 127, 14964-14965.
- Field SJ, Thornton NP, Anderson LJ, Gates AJ, Reilly A, Jepson BJ, Richardson DJ, George SJ, Cheesman MR, Butt JN. (2005) Reductive activation of nitrate reductases. *Dalton Trans.* 21, 3580-3586.
- Hatzixanthis K, Oubrie A, Richardson DJ, Sargent F. (2005) Signal peptide recognition in redox protein maturation. *Proceedings of the National Academy of Sciences USA* 102, 8460-8465
- Olmo-Mira F, Richardson DJ, Castillo F, Moreno-Vivian C, Roldan D (2004) NapF is a cytoplasmic iron-sulfur protein required for Fe-S cluster assembly in the periplasmic nitrate. *Journal of Biological Chemistry* 279, 49727-35
- Clarke TA, Dennison V, Seward HE, Burlat B, Cole JA, Hemmings AM, Richardson DJ (2004) Purification and spectropotentiometric characterization of *Escherichia coli* NrfB, a decaheme homodimer that transfers electrons to the decaheme periplasmic nitrite reductase complex. *Journal of Biological Chemistry* 279,41333-41339
- Jepson B, Anderson L, Rubio L, Taylor C, Butler C, Herrero A, Flores E, Butt JN, Richardson DJ (2004) Tuning a nitrate reductase for function: the first spectropotentiometric characterization of a bacterial assimilatory nitrate reductase reveals novel redox properties. *Journal of Biological Chemistry* 279,32212-32218
- Gronberg K, Thomson AJ, Watmough NJ, Richardson DJ, Field SJ (2004) Redox-dependent open and closed forms of the active site of the bacterial respiratory nitric oxide reductase revealed by cyanide binding studies. *Journal of Biological Chemistry* 279, 17120-17125
- Jormakka M, Richardson DJ, Byrne B, Iwata S (2004) The Architecture of NarGH reveals a structural classification of MGD enzymes. *Structure* 12, 95-104
- Pitts K, Dobbin PSD, Reyes-Ramirez F, Thomson AJ, Richardson DJ, Seward H (2003) Characterization of the *Shewanella oneidensis* MR-1 decaheme cytochrome MtrA: expression in *Escherichia coli* confers the ability to reduce soluble Fe(III) chelates. *Journal of Biological Chemistry* 278,27758-27765
- Reyes-Ramirez F, Sawers RG, Richardson DJ (2003) Characterisation of the transcriptional regulation of *Shewanella frigidimarina* iron-induced flavocytochrome *c* reveals a novel iron-responsive gene regulation system. *Journal of Bacteriology* 185,4564-4571
- Oubrie A, Field SJ, Maritt S, Thomson AJ, Richardson DJ (2002) Spectroscopic characterisation of the soluble NorC domain of bacterial nitric oxide reductase. *Biochemistry* 41, 10858-10865
- Poock SR, Leach, ER, Moir JWB, Cole JA, Richardson DJ (2002) The respiratory detoxification of nitric oxide by *Escherichia coli*. *Journal of Biological Chemistry* 277:23664-23669
- Field SJ, Prior L, Roldan MD, Cheesman MR, Thomson AJ, Spiro S, Butt JN, Watmough NJ, Richardson DJ (2002) Spectral properties of bacterial nitric oxide reductase: Resolution of pH dependent forms of the active site heme *b₃*. *Journal of Biological Chemistry* 277:20146-20150
- Angrove H, Cole JA, Richardson DJ, Butt JN (2002) Protein film voltammetry reveals distinctive fingerprints of nitrite and hydroxylamine reduction by a cytochrome *c* nitrite reductase. *Journal of Biological Chemistry* 277,23374-23381
- Bamford V, Angrove H, Seward H, Butt JN, Cole JA, Thomson AJ, Hemmings AH, Richardson DJ (2002) The structure and spectroscopy of the cytochrome *c* nitrite reductase of *Escherichia coli*. *Biochemistry* 41,2921-2931
- Richardson DJ, Sawers G (2002) PMF through the redox loop. *Science* 295, 1842-1843

COLLABORATORS

Stuart Ferguson (Oxford, UK); Clive Butler (Exeter, UK), Jeff Cole (Birmingham, UK), Megan Maher (Sydney, Aus); Stephen Spiro (Dallas, Texas, US); Maria Delgado (Granada, Spain), Lola Roldan, Cordoba, Spain); Jorg Simon, (Frankfurt, Germany); Jim Fredrickson, John Zacchara (PNNL, Washington, US); Ming Tien, Susan Bradley (Penn State, US)

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EDUCATION

1983 B.S., Biology; Lebanon Valley College
1990 Ph.D., Marine-Estuarine Environmental Science; University of Maryland
1990-1992 NRC Postdoc, Water Resources/Microbial Geochemistry, U.S. Geological Survey
1993 DOE Postdoc, Earth Science/Microbial Geochemistry; Pacific Northwest National Laboratory

EMPLOYMENT

2005- Professor of Geology and Geophysics, University of Wisconsin-Madison
2004-2005 Professor of Biological Sciences, The University of Alabama
1998-2004 Associate Professor of Biological Sciences, The University of Alabama
1993-1998 Assistant Professor of Biological Sciences, The University of Alabama
1993 U.S. DOE Postdoctoral Research Associate, Pacific Northwest National Laboratory
1990-1992 National Research Council Postdoctoral Research Associate, U.S. Geological Survey
1987-1990 Research Assistant, University of Maryland, Chesapeake Biological Laboratory
1986-1987 Teaching Assistant, University of Maryland, Department of Microbiology
1984-1986 Research Assistant, University of Maryland, Chesapeake Biological Laboratory
1982-1983 Research Technician, Pennsylvania Department of Agriculture

PUBLICATIONS (*Five most closely related to the proposed research*)

Roden, E.E. (2008) Microbiological controls on geochemical kinetics, p. 335-467 In *Kinetics of Water-Rock Interactions*. Brantley, S.L., Kubicki, J., and White, A.F. (eds). New York: Springer.
Roden, E.E., and Emerson, D. (2007) Microbial metal cycling in aquatic environments, p. 540-562 In *Manual of Environmental Microbiology, 3rd Edition*. Washington, DC: American Society for Microbiology.
Weber, K.A. P.F. Churchill, K.K. Kukkadapu, and E.E. Roden. 2006. Anaerobic redox cycling of iron by freshwater sediment microorganisms. *Environ. Microbiol.* 8:100-113.
Roden, E.E., D. Sobolev, B. Glazer, and G.W. Luther. 2004. Potential for microscale bacterial Fe redox cycling at the aerobic-anaerobic interface. *Geomicrobiol. J.* 21:379-391.
Sobolev, D., and E.E. Roden. 2002. Evidence for rapid microscale bacterial redox cycling of iron in circumneutral environments. *Anton. van Leeuw.* 81:587-597.

Five other relevant publications

Crosby, H.A., C.M. Johnson, E.E. Roden, and B.L. Beard. 2007. The mechanisms of iron isotope fractionation produced during dissimilatory Fe(III) reduction by *Shewanella putrefaciens* and *Geobacter sulfurreducens*. *Geobiology.* 5:169-189.
Roden, E. E. 2006. Geochemical and microbiological controls on dissimilatory iron reduction. *C.R. Geosci.* 338:456-467. (11, 12) (PDF)
Chandler D.P., Jarrell A.E., Roden E.R., Golova J., Chernov B., Schipma M.J., Peacock A.D., and Long P.E. 2006. Suspension array analysis of 16S rRNA from Fe- and SO₄²⁻-reducing bacteria in uranium-contaminated sediments undergoing bioremediation. *Appl. Environ. Microbiol.* 72: 4672-4687.
Scheibe, T.D., Fang, Y., Murray, C.J., Roden, E.E., Chen, J., Chien, Y.J, Brooks, S.C., Hubbard, S.S. 2006. Transport and biogeochemical reaction of metals in a physically and chemically heterogeneous aquifer. *Geosphere.* 2: 220-235.

Roden, E.E. and T.D. Scheibe. 2005. Conceptual and numerical model of uranium(VI) reductive immobilization in fractured subsurface sediments. *Chemosphere*. 59:617-628.

SYNERGISTIC ACTIVITIES

Editorial board: *Geomicrobiol. J.*, *Geobiology*, *Microb. Ecol.*

Ad-hoc reviewer: *Appl. Environ. Microbiol.*, *Appl. Geochem.*, *Biogeochemistry*, *Environ. Sci. Technol.*, *FEMS Microb. Ecol.*, *Geochim. Cosmochim. Acta*, *Limnol. Oceanogr.*

Environmental Science and Technology, Excellence in Review Award, November 2003

COLLABORATIONS (*Collaborators and Co-Editors*)

Jillian F. Banfield, University of California, Berkeley

Mark O. Barnett, Auburn University

Brian Beard, University of Wisconsin-Madison

William D. Burgos, The Pennsylvania State University

Darryl P. Chandler, Akonni Biosystems

Brian A. Dempsey, The Pennsylvania State University

David Emerson, Bigelow Marine Laboratory

Yuri A. Gorby, Venter Institute

Cindy Gilmour, Smithsonian Environmental Research Center

Clark Johnson, University of Wisconsin-Madison

Derek R. Lovley, University of Massachusetts, Amherst

George W. Luther, University of Delaware

Christopher J. Murray, Pacific Northwest National Laboratory

Flynn Picardal, Indiana University

Nita Sahai, University of Wisconsin-Madison

Timothy Scheibe, Pacific Northwest National Laboratory

Gour-Tsyh (George) Yeh, University of Central Florida

Huifang Xu, University of Wisconsin-Madison

John M. Zachara, Pacific Northwest National Laboratory

Graduate and Postdoctoral Advisors

Graduate: Jon H. Tuttle, University of Maryland, Chesapeake Biological Laboratory

Postdoctoral: Derek R. Lovley, Water Resources Division, U.S. Geological Survey; now in Department of Microbiology, University of Massachusetts, Amherst; John M. Zachara, Pacific Northwest National Laboratory

Thesis Advisor and Postgraduate-Scholar Sponsor

Thesis (8 total):

Jennifer Edmonds, M.S., May 1996

Colin Jackson, Ph.D., Aug 1999

Robert Howell, M.S., May 1999

Dmitri Sobolev, Ph.D., Dec 2001

Karrie Weber, Ph.D., May 2002

Heidi Crosby, M.S. Dec 2006

George Tangalos, Ph.D. Sep 2005-present

Tao Wu, Ph.D. Sep 2006-present

Postgraduate (12 total):

Michael R. Leonardo, Jul 1997-May 2000

Marcie L. Baer, Nov 1998-Jul 2000

Donald Obenhuber, Aug 2002-Apr 2003

Kim A. Warner, Oct 1999-Aug 2004

Byong-Hun Jeon, Jun 2002-Mar 2004

Chris Kennedy, May 2006-Mar 2007

Aaron Coby, Aug 2005-Jul 2007

Marco Blöthe, Sep 2004-present

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John Moreau, Sep 2006-present

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EDUCATION

B.S. 1979 University of Jordan, Amman/Jordan
M.S. 1985 University of Wisconsin-Milwaukee,
Ph. D. 1988 University of Wisconsin-Milwaukee,

AWARDS

9/1975-6/1979: Scholarship, Ministry of Education, Amman, Jordan
8/1984-9/1988: Fellowship, AMIDEAST, Washington, D.C.

PROFESSIONAL EXPERIENCE

2003-present Associate Professor, Dept. of Biological Sciences (UWM)
1998-2003 Assistant Professor, University of Wisconsin-Milwaukee
1995-1998 Assistant Professor, University of Massachusetts at Amherst
1992-1995 Assistant Scientist, Center for Great Lakes Studies, UWM

PUBLICATIONS

- Marshall MJ, Plymale AE, Kennedy DW, Shi L, Wang Z, Reed SB, Dohnalkova AC, Simonson CJ, Liu C, Saffarini DA, Romine MF, Zachara JM, Beliaev AS, Fredrickson JK. 2007. Hydrogenase- and outer membrane c-type cytochrome-facilitated reduction of technetium(VII) by *Shewanella oneidensis* MR-1. *Environ Microbiol.* Sep 20; [Epub ahead of print].
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COLLABORATORS

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EDUCATION

University of Paris 7, Ph.D., 1991, Geophysics
Utrecht University, MS, 1988, Geophysics
Utrecht University, BS, 1984, Geophysics

EXPERIENCE

Dr. Versteeg's research focuses on experimental near surface geophysics. He has done extensive research in the application of numerous geophysical methods to image hydrological and biogeochemical processes, and has designed and implemented several laboratory and field scale autonomous geophysical acquisition systems. Research efforts included also the development of inverse methodologies and coupled hydrologic/geophysical modeling research.

Part of his recent research has focused on the design and implementation of systems to deliver information in near real time over the web, and on the design and implementation of scientific work flow systems for auditable result generation and delivery, specifically in the area of performance monitoring. This also includes research in the automation of geophysical data acquisition, both for static systems and for robotically deployed systems. Dr. Versteeg operates a laboratory for geophysical characterization of cores and columns, and has access to a comprehensive geophysical field instrumentation pool and runs a laboratory for laboratory scale investigation of electrical geophysical signatures. He currently is receiving funding from the Department of Energy, Department of Defense and the Environmental Protection Agency for a range of monitoring projects.

PROFESSIONAL AFFILIATIONS

- American Geophysical Union
- Society of Exploration Geophysicst
- European Association of Geoscientists and Engineers
- Environmental and Engineering Geophysical Society

RELEVANT PROFESSIONAL ACTIVITIES

- Associate Research Scientist/Adjunct Assistant Professor, Lamont Doherty Earth Observatory/Columbia University, 1995-2001
- Past associate editor of Geophysics
- Head of INL Geophysical Monitoring Group (2002-present)
- Visiting Scientist at TNO Netherlands (March 2007-August 2007)

SELECTED PUBLICATIONS

Wu, Y., Slater, L., Versteeg, R. and LaBrecque, D., 2008, A comparison of the low frequency electrical signatures of iron oxide versus calcite precipitation in granular zero valent iron columns, *Journal of Contaminant Hydrology*, volume 95 (3-4): 154-167.

Versteeg, R., A. Richardson and T. Rowe (2006). Web accessible scientific workflow system for performance monitoring. *Environmental Science and Technology* 10.1021/es0517421 S0013-936X(05)01742-6.

- Zheng, Y., A. Van Geen, M. Stute, R. Dhar, Z. Mo, Z. Cheng, A. Horneman, I. GAVRIELI, H. J. Simpson, R. Versteeg, M. Steckler, A. Graziolo-Venier, S. Goodbred, M. Shahnewaz, M. Shamsudduha, M. A. Hoque and K. M. Ahmed (2005). "Geochemical and Hydrogeological Contrasts between Shallow and Deeper Aquifers in Two Villages of Araihasar, Bangladesh: Implications for Deeper Aquifers as Drinking Water Sources." *Geochimica et Cosmochimica Acta* **69**(22): 5203-5218
- Versteeg, R. et al., 2004. A structured approach to the use of near surface geophysics in long term monitoring. *The Leading Edge*, 23(7): 700-703.
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- Sandberg, S., L. Slater and R. Versteeg (2002). "An integrated geophysical investigation of the hydrogeology and an anisotropic unconfined aquifer." *Journal of Hydrology* **267**: 227-243.
- Slater, L., A. Binley, R. Versteeg, G. Cassiani, R. Birken and S. Sandberg (2002). "A 3D ERT study of solute transport in a large experimental tank." *Journal of Applied Geophysics* **49**(4): 211-229.
- Birken, R. and Versteeg, R., 2000. Use of four dimensional ground penetrating radar and advanced visualization methods to determine subsurface fluid migration. *Journal of Applied Geophysics*, 43: 215-226.
- Versteeg, R. and Gochioco, L. (guest editors), 1999, Special Issue on engineering geophysics of The Leading Edge (December 1999 Issue).
- Sato, M. and Versteeg, R. (editors), 1998, Special Issue on ground penetrating radar of the *Journal of Applied Geophysics*, Vol 40, 1-3.
- Versteeg, R. and Grau, G. (editors), 1991, The Marmousi experience, proceedings of the 1990 EAEG workshop on practical aspects of seismic data inversion, EAEG, Zeist.

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EDUCATION

1999 University of California, Davis Ph.D. (Civil Engineering)
1991 Washington State University M.S. (Environmental Engineering)
1988 Washington State University B.S. (Civil Engineering)

EXPERIENCE

Associate Professor, 2005-Present; School of Chemical, Biological, and Environmental Engineering, Oregon State University
Assistant Professor, 2001-2005; Department of Civil, Construction, and Environmental Engineering, Oregon State University
Senior Research Scientist, 1994-2001; *Research Scientist*, 1990-1994; Pacific Northwest National Lab, Richland, WA

My expertise is in transport theory and experimental methods for studying transport in multiphase, reactive media. My research has been centered around engineering problems that require the upscaling of interacting physical, biological, and chemical systems; particular focus has been on problems involving reactive solute transport in porous media. A variety of theoretical techniques have been explored during this research, including classical ensemble averaging, field-theoretical methods for upscaling, and volume averaging. Applications that I have worked on include the development of effective transport theories for (1) reactive solutes in porous media under transient flow conditions, (2) biologically active compounds in biofilms and tissues, and (3) chemicals undergoing catalytic transformations in spatially heterogeneous catalysts. Recent efforts have involved the use of the method of volume averaging with closure, with closure being accomplished in realistically structured periodic unit cells in 3-dimensions.

A significant component of my research has been directed toward efforts to corroborate theory (facilitated, usually, by high-performance computational tools) and data from experiments or applications. I have extensive experience in conducting flow and transport experiments in porous media, with a focus on problems that involve reactions.

SELECTION OF RECENT PUBLICATIONS

- Chastanet, J. and B. D. Wood, 2008. The mass transfer process in a two-region medium, *Water Resources Research*, in press.
- Wood, B.D., 2007. Inertial effects in dispersion in porous media, *Water Resources Research*, 43, W12S16, doi:10.1029/2006WR005790.
- F. Golfier, Quintard, M., Cherblanc, F., Zinn, B.A., and Wood, B.D., 2007. Comparison of theory and experiment for solute transport in highly heterogeneous porous medium, *Advances in Water Resources*, 30: 2235-2261.
- Wood, B.D., K. Radakovich, and F. Golfier, 2007. Effective reaction at a fluid-solid interface: Applications to biotransformation in porous media, *Advances in Water Resources*, 30: 1630-1647.
- Wood, B.D. and R.M. Ford, 2007. Editorial: Biological processes in porous media: From the pore scale to the field, *Advances in Water Resources*, 30: 1387-1391.

- Ramirez, J. M., E. Thomann, E.C. Waymire, J. Chastanet, and B. D. Wood, 2007. A Note on the Theoretical Foundations of Particle Tracking Methods in Heterogeneous Porous Media, in review for *Water Resources Research*.
- Tartakovsky, A. M., P. Meakin, T.D. Scheibe, and B. D. Wood, 2007. A smoothed particle hydrodynamics model for reactive transport and mineral precipitation in porous and fractured media, *Water Resources Research*, 43, doi:10.1029/2005WR004770.
- Wood, B.D., F. Cherblanc, M. Quintard, and S. Whitaker, 2003. Volume averaging for determining the effective dispersion tensor: Closure using periodic unit cells and comparison with ensemble averaging, *Water Resour. Res.*, 39: 10.1029/2002WR001723.
- Scheibe, T. D., and B. D. Wood. 2003. A Particle-Based Model of Size or Anion Exclusion with Application to Microbial Transport in Porous Media. *Water Resour. Res.*, 39: doi:10.1029/2001WR001223.
- Wood, B.D., M. Quintard, and S. Whitaker, 2002. Calculation of effective diffusivities for biofilms and tissues, *Biotechnology and Bioengineering*, 77, 495-516.

SYNERGESTIC ACTIVITIES

Courses Taught: Fluid Mechanics for Chemical Engineers; Environmental Engineering Design, emphasizing 'guided design'; Upscaling methods in Engineering. **Manuscript Reviews:** *Water Resources Research*, *Advances in Water Resources*, *Transport in Porous Media*, *Biotechnology and Bioengineering*. **Editorial Board:** Guest Editor for *Advances in Water Resources*. **Professional Memberships:** American Geophysical Union (AGU), American Institute of Chemical Engineers (AIChE), American Association for the Advancement of Science (AAAS), United Nations Association of the USA (UNA-USA), International Water Association (IWA)

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