U.S. DEPARTMENT OF ENERGY

PNNL-SA-96928

Prepared for the U.S. Department of Energy
under Contract DE-AC05-76RL01830

PNNL Scientific Focus Area: Hydro-Biogeochemical Process Dynamics in the Groundwater-Surface Water Interaction Zone

Principal Investigators:
J. M. Zachara J. K. Fredrickson

Laboratory Research Manager
C. A. Geffen

July 2013

Pacific Northwest NATIONAL LABORATORY

Proudly Operated by Battelle Since 1965

PACIFIC NORTHWEST NATIONAL LABORATORY
operated by
BATTELLE
for the
UNITED STATES DEPARTMENT OF ENERGY
under Contract DE-AC05-76RL01830

PNNL SBR Scientific Focus Area Annual Report FY2013

Hydro-Biogeochemical Process Dynamics in the Groundwater-Surface Water Interaction Zone

2013 Annual Report
July 12, 2013

Table of Contents

I. Program Overview

The PNNL SFA is investigating biogeochemical transport and microbiological processes in a hydrologically dynamic and interactive groundwater-surface water system near the Columbia River shoreline at the southern end of the Hanford Site. Research quantifies elemental biogeochemical processes (C, N, Fe, Mn, S, U, and Tc) that occur in the field, identifies the ecologic and hydro-geologic properties and phenomenon that control them, tests field-driven hypotheses in the laboratory across molecular to core scales, and develops new models to describe how interactions in this zone influence chemical fluxes to surface waters and larger system behaviors. We focus on the GWSWIZ because it is a poorly understood hydro-biogeochemical domain present in all watersheds that is not generally represented in land surface models. It is a uniquely dynamic and reactive zone through which large volumes of surface water re-circulates and mixes with groundwater, and where diverse and active microbial communities exist in association with particle surfaces. Biogeochemical reactions in the GWSWIZ: 1.) control the fluxes of groundwater contaminants to surface waters, and 2.) influence the carbon and nitrogen budgets of watersheds both large and small.

Field investigations including microbial activity and genomic analyses, down-well microcosm studies, and time series monitoring of key hydrologic and chemical parameters in different hydrogeologic zones of the system seek to identify: i.) biotic and abiotic variables diagnostic of integrated system function, and ii.) emergent behaviors when, if, and where they occur. The 300 Area field site is scientifically rich and includes an oxic uranium-containing vadose zone and groundwater plume, a deep underlying stratigraphic sequence of naturally reduced sediments with variable hydraulic properties, oxic and anoxic groundwater-river mixing zones extending up to 250 m inland, and a biologically active hyphoreic zone with oscillatory water flow vectors. Ongoing field studies seek to understand and model an approximate 0.1 km^2 domain within the interaction zone, with larger scales to be addressed in the future.

Integrative data assimilation methods that identify and propagate uncertainty, multi-scale stochastic biogeochemical transport modeling, and statistically-based microbial ecologic modeling are applied iteratively with experimentation to: i.) build integrated system simulators of increased accuracy, and ii.) identify hierarchical process interactions controlling system behavior. The development of an improved biogeochemical transport model that integrates molecular information on microorganism phylogeny and function with community spatial distribution and ecology is a long-term goal. Models are applied in the design of field experiments to investigate system behavior, to integrate multi-process information and characterization data, and to understand and predict large-scale behaviors of the 300 A groundwater-surface water interaction zone.

Contaminant uranium is a reactive hydrochemical tracer in the oxic zone and underlying redox transition zone sediments, and its complex hydrochemical behavior in association with that of carbon provides unique insights on multi-process interactions that change on a seasonal basis. The in-situ microbial community, and its function and response to dynamic hydrochemical conditions, is investigated through a combination of 16s-RNA sequencing, single cell genomics, and metagenomics with exploratory proteomics investigations underway. Large integrative experiments monitor spatio-temporal trends in subsurface microbial ecology, terminal electron acceptor concentrations, metabolic activity, and dissolved U concentrations associated with seasonal Columbia River intrusion to resolve hypotheses on elemental cycling and fluxes, carbon sources, microbial ecosystem homeostatsis, and emergent system behaviors. Key microscopic reactive transport mechanisms that must be understood to predict field behaviors are evaluated in the laboratory using site-derived microorganisms and sediments, and abstracted model biogeochemical systems.

Our integrated multi-scale experimental and modeling approach, driven by field scale observations and the identification and prediction of system scale diagnostic variables using coupled process models with mechanistic integrity, fully supports the four long term goals (7-10 y) of the 2012 CESD Strategic Plan.

II. Goals, Science Questions, and Objectives

The PNNL SBR-SFA is pursuing three primary goals:

- To understand the holistic biogeochemical functioning of the groundwater-surface water interaction zone as it influences contaminant fate and transport, carbon and nitrogen fluxes, and land surface responses to climate change,
- To determine how the coupling of hydrophysical, microbiologic, and geochemical processes controls elemental biogeochemical cycling at different scales in the groundwater-surface water interaction zone, and
- To develop an open source, multi-scale data assimilation and modeling framework that predicts system scale microbiologic and geochemical behaviors and fluxes for subsurface water systems influenced by groundwater-surface water exchange, microenvironments, and redox transition zones.

The following broad science questions motivate current research:

- What are the primary biogeochemical pathways mediated by microorganisms in the Columbia River GWSWIZ, and what are their electron donors [e.g., recent or ancient carbon, or lithogenic Fe(II)] and acceptors [e.g., NO_3^-, Fe(III) oxide, Fe(III) clay]?
- What is the spatial and depth distribution of biogeochemical function, what are the controlling environmental factors, and how does community structure and function respond to dynamic hydrologic events such as river water intrusion and retreat?
- What chemical and microbiological signatures present in either sediment or water are diagnostic of system behavior?
- How can biogeochemical process measurements and models developed through laboratory scale experimentation be applied at the km scale, or are large system behaviors emergent?

- How is genomic information on the mediated biogeochemical reaction networks, the community structure and its temporal variations, and controlling subsurface properties best integrated to predict system behavior and diagnostic signatures at the km scale?

Research Theme Areas

The project is divided into three interactive theme areas (Figure 1) with the following objectives:

Theme Area I: Complex System Analysis and Multi-Scale Models

Objective: Apply new data assimilation methods to integrate multi-disciplinary field data and microbiologic analyses, and their uncertainties, into a biogeochemical transport model for iterative experimental design and multi-scale/field system predictions of solute and gas fluxes and their spatial and temporal distributions. Investigate the coupling of transport and biogeochemical reaction processes from the microenvironment (e.g., grain) to the field scale to identify emergence when it occurs, and the factors responsible for process and parameter scale-dependency. Conceptualize and apply innovative geostatistical and phenomenological models for complex system analysis that are free from reductionistic constraints. Participate in the development of SBR community models for integrated watershed system science with other lab SFAs.

Theme Area II: Field Experiments in the GWSRIZ

Objective: Quantify the biogeochemical functioning of oxic and reduced groundwater – surface water interaction zones through time series measurements of solutes (emphasizing C, N, S, U, and Fe) and microorganisms in groundwater and associated sediments as a function of depth, distance from the river, and groundwater-river water mixing ratio. Utilize geophysical measurements to map subsurface structures and quantify spatio-temporal dynamics of river water intrusion and retreat. Determine microbial community structure and function in space and time using metagenomics and single-cell sequencing approaches; and establish relationships to hydrochemical variables and aquifer hydrophysical properties through geostatistical analyses. Determine the nature and reactivity of carbon sources and inorganic electron donors driving the subsurface biogeochemical processes. Employ other field experiments to assess in-situ activities, functionality, and biogeochemical process rates and their spatio-temporal variability.

Theme Area III: Functional Analyses and Process Models

Objective: Through laboratory study, identify the mechanisms and fundamental reaction rates of key biologic, geochemical, and biogeochemical reactions necessary to predict system behavior at the field scale. Identify community taxonomy and active gene functions in spatio-temporal samples via high-throughput 16s RNA sequencing and metagenomics, and verify key predicted metabolic activities and reaction networks through laboratory manipulation of field derived microbial isolates and consortia. Investigate the coupling of transport and biogeochemical reaction processes from the microenvironment scale (e.g., grain) to the macroscopic scale using site sediments and microorganisms to develop process models and reaction parameters for up-scaling and identification of emergent behaviors. Link microscopic and macroscopic findings to

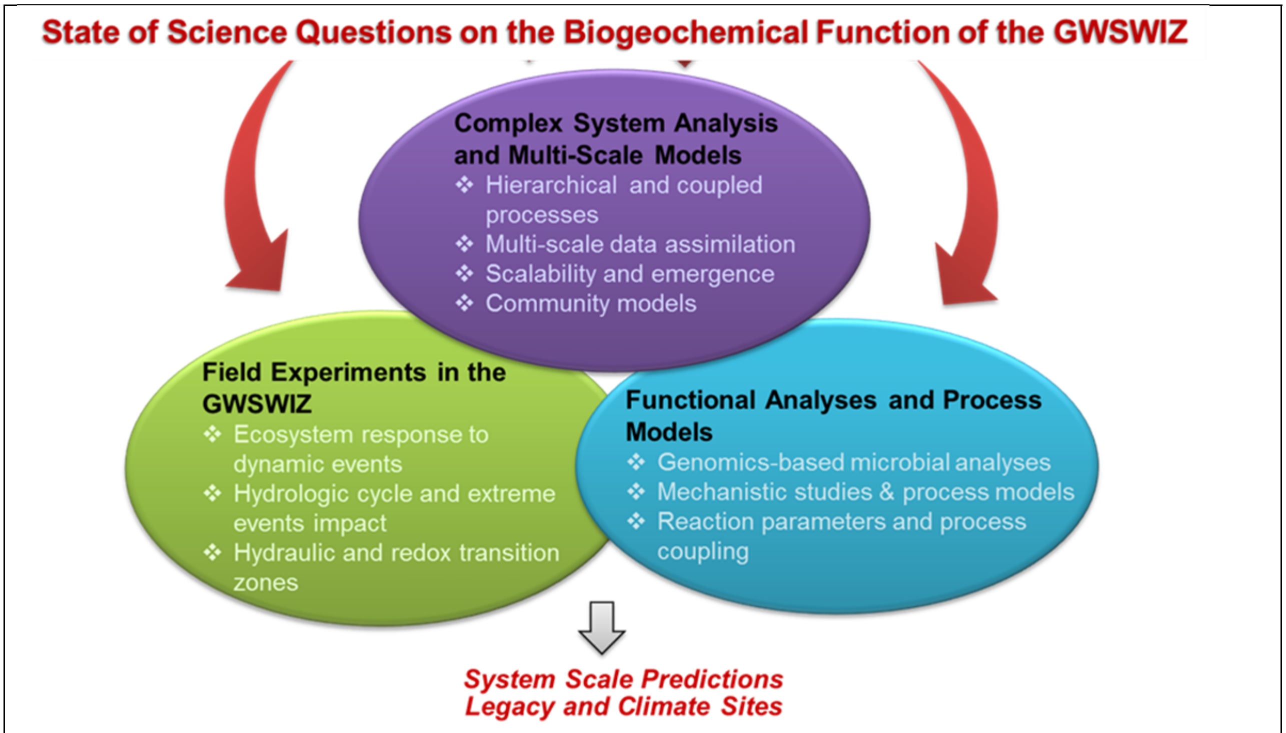

Figure 1. Science theme structure of the PNNL SBR SFA. Within this structure model needs inform field hypotheses while targeted new observations improve models. Field questions and system modeling needs drive laboratory studies and the development of process models.

the field scale through more accurate, but pragmatic process representations in higher scale biogeochemical transport models.

III. Program Structure

SFA Management

Charlette Geffen – Laboratory Research Manager. Communication and coordination of overall research directions and scientific impact with SBR/BER management
Jim Fredrickson – Scientific manager. Set research directions, milestones, and funding in alignment with SBR strategic plans and guidance. Encourage P.I. collaborations and synergies. Lead on all biologic research.
John Zachara – Scientific manager. Set research directions, milestones, and funding in alignment with SBR strategic plans and guidance in collaboration with JF. Encourage P.I. collaborations and synergies. Lead on all chemical and physical sciences research.

Theme Area I: Complex System Analysis and Multi-Scale Models

Xingyuan Chen – Research contributor in data assimilation, uncertainty analysis, stochastic transport modeling, and complex systems models.

Glenn Hammond – Research lead in high performance computing, PFLOTRAN, hydrologic processes, large system simulations, and open source code development.
Chris Murray **–** Research contributor in geo-statistics and complex system analysis.
Chongxuan Liu – Research lead on biogeochemical transport model development and parameterization. Linkage with CLM and new community land models

Theme Area II: Field Experiments in the GWSRIZ

Allan Konopka – Research lead on field studies of microbial ecology.
Jim McKinley – Research contributor in field geochemistry
Jim Fredrickson **–** Contributing P.I. with focus on biogeochemistry and elemental transformations across 300 A redox transition zones.
Tim Johnson – Research contributor with expertise in field geophysical measurements and inversion modeling.
James Stegen **–** Contributing young scientist in field microbial ecology, and ecological modeling (New hire in CY 2013).
Mike Wilkins – Contributing young scientist in field biogeochemistry, proteomics, and single-cell genomics (leaving lab in 7/2013).

Theme Area III: Functional Analyses and Process Models
.
Kevin Rosso – Research lead on molecular biogeochemistry including electron transfer modeling in biotic and abiotic systems.
Liang Shi **–** Contributing P.I. on molecular biochemistry including protein expression, isolation, characterization, and mechanistic reaction studies in collaboration with external P.I. Richardson.
Andy Felmy – Contributing P.I. with focus on actinide biogeochemistry and project-wide applications of thermodynamic modeling.
Bill Nelson **–** Research contributor with focus on metagenomics and bioinformatics (New hire in CY 2012).
Tim Scheibe – Research contributor with focus on pore scale modeling and up-scaling.
John Zachara – Contributing P.I. with focus on biogeochemical process characterization in sediments.

IV. Performance Milestones and Metrics

Scientific Progress

Here we summarize select progress for the three theme areas. Size constraints preclude a comprehensive report. Two major cross theme field experiments were initiated during the reporting that represent important project metrics for FY 2013. These experiments integrate the research activities of all SFA participants through closely coordinated field, modeling, and laboratory activities. Progress will described in the context of these two field activities as these represent our future direction. Our publications (**Appendix A**) are another important metric of performance.

A. Experiment I – Columbia River Intrusion and Retreat

Objective: Assess the stability of subsurface microbial community structure and function to hydrochemical change driven by natural seasonal variations in Columbia River stage.

Primary Hypotheses: River water intrusion is controlled by hydrogeologic structures. Intrusion introduces metabolizable solutes (particulate and dissolved organic carbon) and allochtonous microorganisms that compete with and displace indigenous members, shifting community composition and function.

Approach and Staff Interactions: The experiment involves the monitoring and sampling of an approximate 300 m x 300 m x 8 m subsurface domain located along and inland of the Columbia River shoreline for a six-month time period (April-September 2013). The domain straddles a buried subsurface channel that is believed to facilitate groundwater-river exchange (Figure 2). The dynamic intrusion and retreat of Columbia River water into the unconfined aquifer is being monitored by 3D electrical resistivity tomography (ERT) using a novel time lapse ERT imaging methodology that explicitly accommodates the water table contrast, providing 3D images of river water intrusion at a temporal resolution of three images per day. Samples for aqueous geochemical and microbiological analyses are taken from a transect of wells that begins at the river shoreline, progressing inland along the channel to the IFRC site (Figure 2). Sand packs have been suspended in these same wells to allow sampling of the sediment-bound microbial community.

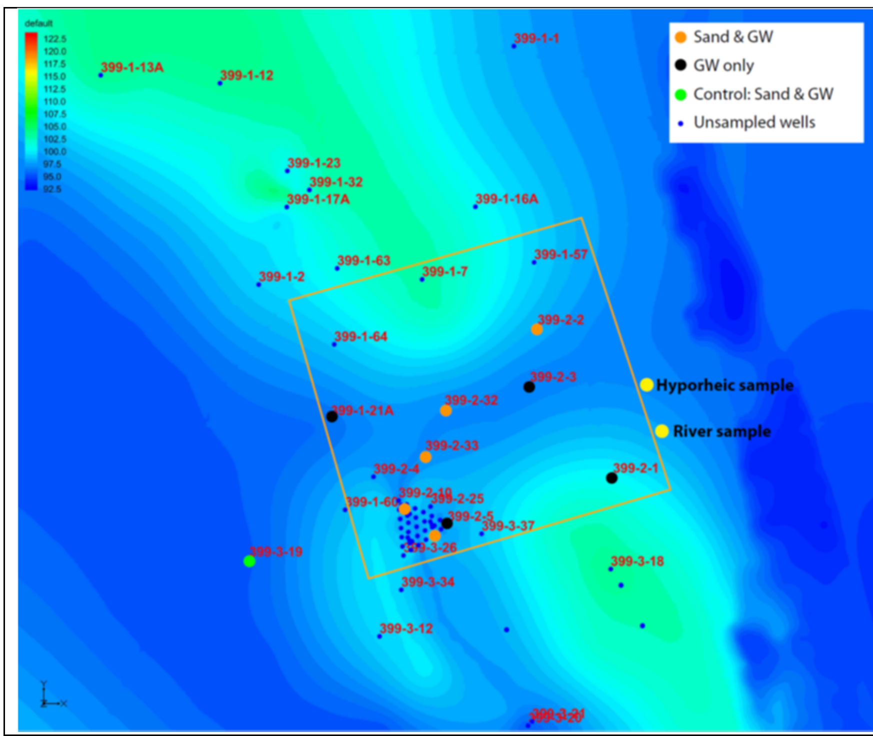

Figure 2. Study area (orange outline, 300 m x 300 m) for the Spring 2013 intrusion experiment. The Columbia River runs along the east margin of the research domain. The IFRC site is located in the south-west corner of the study site.

A wide variety of measurements are being performed to characterize the system response to river water intrusion and retreat. In addition to ERT, the dynamic groundwater – surface water hydrologic interaction is being monitored with an array of continuous pressure, temperature, and specific conductance probes installed in wells. Nine of these wells and the Columbia River gage station have been instrumented with telemetry, and these data are available real-time online with automated alerts to improve the robustness of monitoring equipment and better ensure a complete data package. Groundwater samples are analyzed for inorganic cations and anions, U(VI), carbonate species, and dissolved and particulate organic carbon concentrations. Compositional measurements on the aqueous organic matter fractions are performed with FT-ICR mass spectrometry in EMSL. Cell density measurements by flow cytometry and DNA extractions are used to characterize the planktonic microbial community. Analyses of the sand packs will provide insights on changes to the sediment-bound community. These analyses will include: ATP-based estimation of cell density, tritiated leucine incubation to determine metabolic rate, DNA for amplicon sequencing and shotgun metagenomics, and RNA for rRNA and mRNA sequencing.

The intrusion experiment involves staff from all three theme areas, including Hammond, Chen, and Murray from Theme Area I; Konopka, Stegen, and Johnson from Theme Area II, and Nelson and Zachara from Theme Area III.

Results to Date: The IFRC and SFA projects have been monitoring various aspects of the spring groundwater-river water interaction for 5 yr. The character of spring stage maximum (e.g., duration and magnitude) has been very different each year, and CY 2013 has been no exception. Figure 3 illustrates web-generated plots of the groundwater elevation and specific conductance for the telemetry wells during high river stage to date this year (CY 2013). The plots clearly demonstrate through a drop in specific conductance (well conductivity) during high river and water table elevation that river water intrudes far inland to wells 399-2-32 (yellow), 399-2-33 (magenta) and 399-3-20 (green) located 200-250 meters from the river bank.

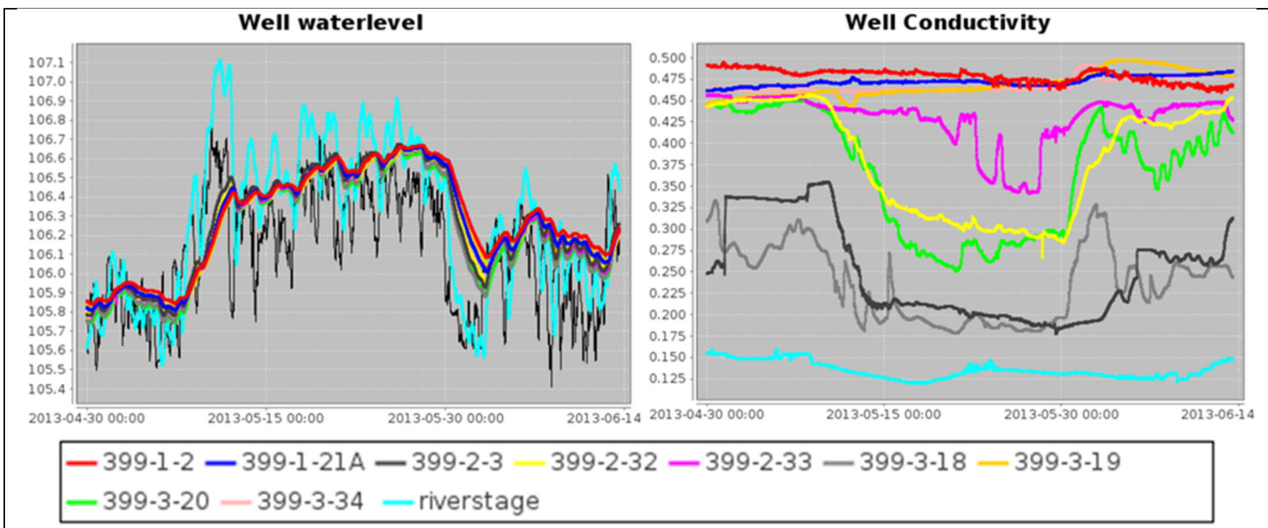

Figure 3. Web-based plots of groundwater elevation and specific conductance (conductivity) for Spring 2013 at telemetry wells within the PNNL SFA field site at the Hanford 300 Area.

ERT imaging of the 300 m x 300 m domain is providing important information on the spatial distribution and residence time of river water in the unconfined aquifer, and its complex and dynamic changes in response to river stage (Figure 4). These results will place the comprehensive geochemical and microbiologic analyses performed on specific well-waters and sand packs in context, providing a link between micro-scale and system scale observations. Ultimately this information will be used to help upscale coincident well-based microbiologic and geochemical measurements to the field scale, and to inform future reactive transport model calibration.

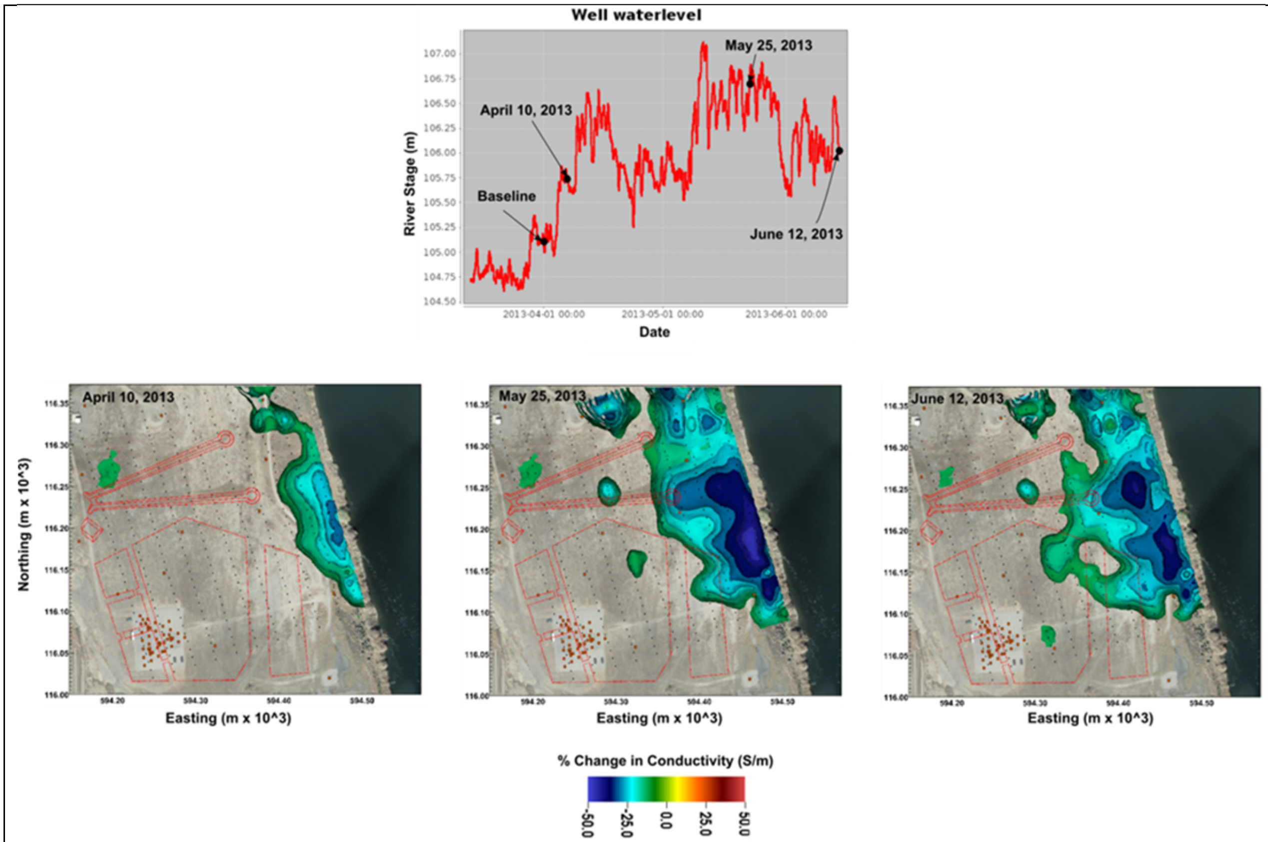

Figure 4. (top) 2013 Columbia River stage level. Black dots show times of ERT images. (bottom) Example time-lapse images of changes in electrical conductivity caused by river water intrusion into the Hanford 300 Area. Conductivity changes are shown as isosurfaces.

To date, 300 well-water and 100 sand pack samples have been collected from the well transect and preserved, with another 200 samples to be collected before experiment completion. Anion and cation, and carbon analyses of groundwaters are underway, as are ATP and leucine measurements of sand pack sediments. Extracted DNA and RNA are being held until all sampling is complete to minimize the effects of analytical variability contributed by multiple sequencing runs.

<u>Next Steps</u>: The initial next step will be to complete all geochemical and microbiologic analyses of well-water and sand pack samples collected during the six-month experiment, and to subject them to multi-level interpretational analyses. The large number of samples collected and

analyzed will lead to a large, multi-component data base with diverse and complex spatio-temporal character. Geostatistical analyses of geochemical and microbiologic data will initially be performed to identify relationships between measured parameters, and parameters diagnostic of system response to river water intrusion and retreat. Bioinformatics analyses of the extensive metagenomics and RNA sequencing data sets on their return will be performed to: i.) assess the structure and function of the subsurface microbial ecosystem and its spatial evolution with distance from the river, and ii.) identify changes driven by river water intrusion and retreat. Metabolic reconstructions based on the sequencing data and geochemical analyses will be used to develop a biogeochemical reaction network for the system that will be integrated (below) into our system-scale simulator. Ecologic modeling will assess the primary ecologic processes governing the observed subsurface ecosystem response, including selection, dispersal, and drift; and identify the controlling environmental factors (e.g., measured parameters) and potentially important unmeasured variables.

The massively parallel flow and transport code PFLOTRAN (Hammond et al, 2012) is being coupled to the parallel geophysics code E4D (Johnson et al., 2010) to provide a multi-physics (fluid flow, solute transport, and current flow) capability to simulate all field hydrologic and transport data from the intrusion experiment. Once well sensor and geophysical data for the complete high-water season (e.g. March-September) have been collected and vetted, this coupled forward model will be employed within a Bayesian data assimilation framework that leverages high performance computing to execute large ensembles of simulations and invert for hydrologic parameters. The optimized hydrologic model will be used as the base flow model for the PNNL SFA's biogeochemical transport modeling effort.

We have also been developing an automated community data assimilation framework, leveraging HPC and community resources, to integrate and model the multiple spatio-temporal data types obtained from the field experiment as described above. This data assimilation and modeling framework will serve as a tool to: i.) test system scale attributes and conceptual models (such as the biogeochemical reaction network and ecosystem spatial structure); ii.) improve the integration between model developments and field data collections; and iii.) quantify the uncertainty of system scale predictions and the reduction in uncertainty provided by new measurements or interpretations. To satisfy the computational demands of this project, an ASCR Leadership Class Challenge (ALCC) supercomputing allocation of 16 million hours was awarded for this modeling effort in May by the DOE Office of Science, and a request for six million additional hours on the BER-funded Chinook supercomputer is currently under review within EMSL.

Expected Contributions: This large multi-disciplinary field experiment will provide the first system scale analyses of a subsurface ecosystem in an oligotrophic groundwater-surface water interaction zone, and the biogeochemical processes that it mediates. Environmental factors controlling the subsurface ecosystem, the ecologic processes involved, and the system responses to dynamic natural events will be determined. The resulting conceptual model will form the basis for a first-of-kind coupled process model of the GWSWIZ whose development will begin in FY2014. The model will include ecologic, microbiologic, biogeochemical, and hydrologic processes to predict fluxes of C, N, nutrients and contaminants at the local and regional scale. The research will also demonstrate a novel inverse method for incorporating geophysical data in hydrologic parameter estimation and result in a publicly available multi-year data package composed of comprehensive geophysical measurements, and associated groundwater elevation, temperature, composition, and biogeochemistry data.

B. Experiment II – Redox Transition Zone Beneath the Oxic U-Plume

Objective: Determine the chemical, microbiologic, and geohydrologic factors controlling the formation and maintenance of an extended and abrupt redox interface in the near-shore unconfined aquifer; the directions and magnitude of biogeochemical fluxes of C, N, S, and Fe; and the microorganisms, electron donors, and electron acceptors that drive system response.

Primary Hypotheses: The distribution of ancient carbon and sediment physical properties controlling oxygen diffusivity determine the spatial distribution of the redox transition zone. Oxidized, soluble N and S species and solid-Fe(III) forms (Fe-phyllosilicates) function as primary electron acceptors. The depth of the redox interface is controlled by the complex interplay of microbial activity, transport processes, and sediment depositional environment controlling the concentrations of soluble and sediment-associated electron donors and acceptors.

Approach and Staff Interactions: This multi-investigator experiment has active field and laboratory components. Field studies include fine scale measurements (every 25 cm) of microorganisms, groundwater solutes, metabolically-reactive ions, and dissolved gases with depth in groundwaters above, within, and below a redox transition zone located immediately proximate to the Hanford-Ringold lithologic contact. The system is monitored through the deployment of 3 m multi-level sampling (MLS) strings that are placed within six different 300 A well bores that vary in sedimentary stratigraphy and redox status. The wells are distributed over an approximate 1 km^2 area. The MLS strings are designed with suspended diffusion cells for collection of dissolved solutes, syringes for collection of dissolved gases (H_2, CH_4, and N_2O), and sand packs for collection of microorganisms. The MLS strings are being deployed for a period of one year with approximate 6 week sampling intervals.

Companion laboratory studies are being performed with intact core samples and sediments collected from four of the wells during their installation. An important objective of these studies is to characterize controlling processes and process interactions as they may occur in the field to provide up-scalable biogeochemical reaction parameters to model field observations and behaviors. Laboratory studies are characterizing important attributes of key system components to allow development of reaction based models, including the composition of organic matter electron donors, the thermodynamic and surface chemical properties of solid phase Fe-phyllosilicate electron acceptors, and the biochemical reaction mechanisms of key microorganisms mediating redox reactions. The sediment hydrologic properties (e.g., hydraulic conductivity and pore size distribution and connectivity) are also considered as essential controls on water, gas, and solute flux. Reactive transport experiments in the lab assess the rates of individual biogeochemical reactions under simulated in-situ conditions as influenced by microbial biomass, sediment properties (e.g., porosity, mineralogic composition), and water flow in order to develop multi-component biogeochemical reaction networks for linkage with transport models.

The redox transition zone experiment involves staff from all three theme areas, including Liu and Murray from Theme Area I; Fredrickson, McKinley, and Stegen from Theme Area II; and Felmy, Nelson, Rosso, Scheibe, and Shi from Theme Area III.

Results to Date: Deployment of the multi-level samplers began in March 2013, so the field campaign is approximately 33% complete as of July 2013. Results of the first sampling revealed a strong biogeochemical reaction signature in well water composition for most of the studied wells (Figure 5). The close vertical spacing of samples and their attendant analyses is an important attribute of the MLS system. The concentrations of nitrate (NO_3^-) decreased, while those of sulfide (S^{2-}) increased dramatically below the Hanford-Ringold contact where the redox transition zone is believed to exist based on sediment coloration. These trends were consistent with the occurrence of microbiologically driven dissimilatory nitrate and sulfate reduction across the transition zone. Organic carbon is typically the electron donor for these biogeochemical reactions. The presence of significant dissolved nitrite (NO_2^-) below the zone of nitrate loss confirmed the presence of denitrification. Analyses of sediment from the zone of high sulfide production (e.g., -0.5 m) revealed the presence of frequent framboidal pyrite (FeS_2), indicating sustained sulfide production, and consequently sulfate reduction, over extended time periods. Mossbauer spectroscopy analyses of sediments below the zone of nitrate reduction revealed the presence of copius Fe(II)-phyllosilicates, evident as terminal products of dissimilatory iron reduction.

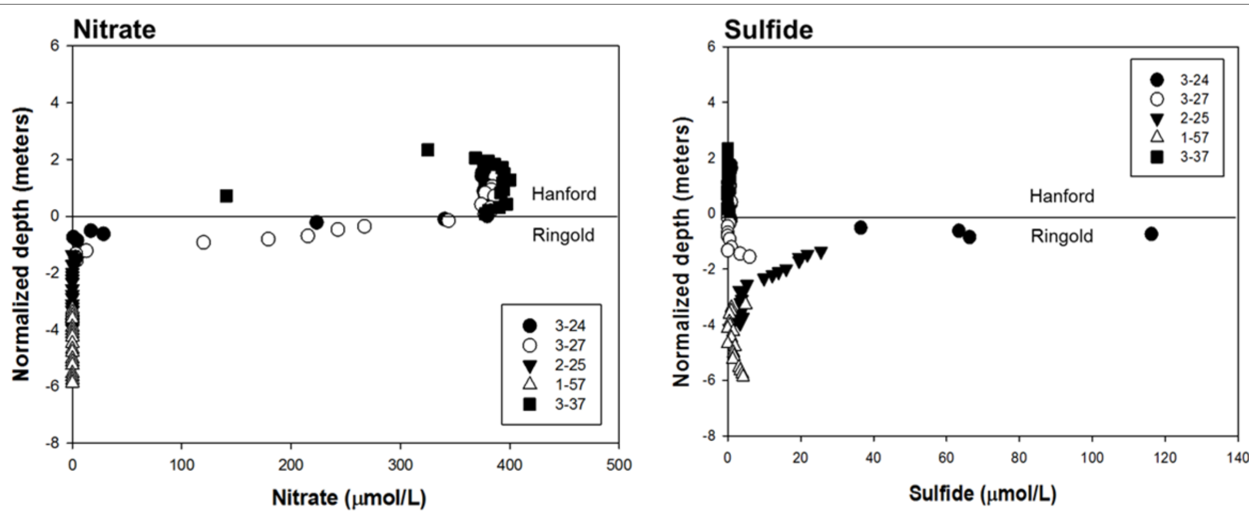

Figure 5. MLS measurements across Hanford/Ringold contact from multiple wells in the first MLS deployment. The depth data on the y-axis is normalized to the Hanford-Ringold contact that occurs at different depths in the different wells. The median depth of this interface is 18 m below ground surface.

Also common to some of the sampled well waters were high concentrations of methane (>10 μmol/L, data not shown). The highest concentrations of methane occurred at or below the Hanford-Ringold contact, but were spatially heterogeneous. The lack of apparent correlation of methane concentrations with the transition zone indicates that methane originates from heterogeneously distributed domains of ancient organic matter at meter plus spacing that are occasionally evident in core samples. 16s-RNA pyrotag sequencing of sediments above, within, and below the transition revealed a complex taxonomic distribution of microorganisms (Figure 6) with high concentrations of methanotrophs observed near the transition zone. These findings suggest that methane cycling is an important process in this system, with potential methane losses to the Columbia River and atmosphere.

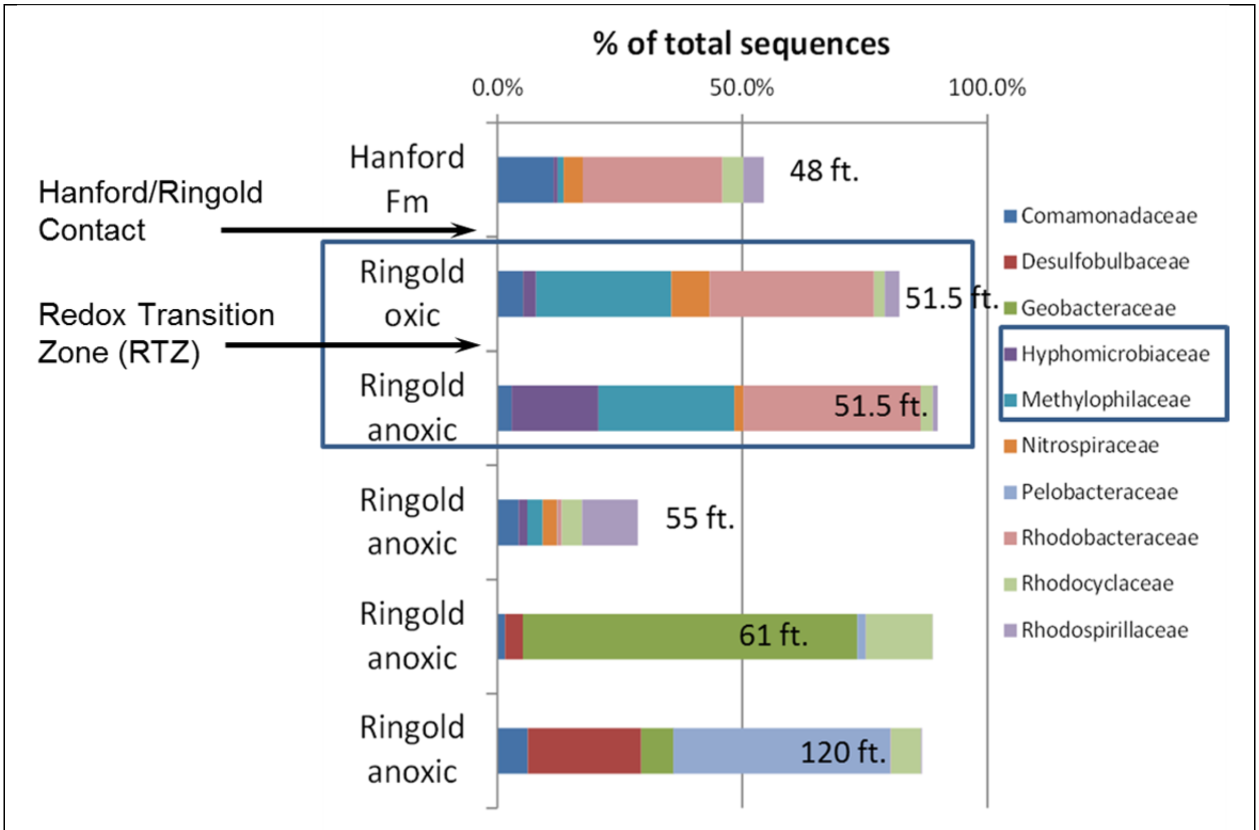

Figure 6. Distribution of microbial taxa above, within, and below the redox transition zone. Hyphomicrobiaceae and Methylophilaceae are methanotrophs.

Significant progress has also been made on the laboratory component of the study to identify and quantify key reaction mechanisms and processes controlling field behavior. Briefly, this has included four primary activities: 1.) Quantifying dentrification rates in sediments across the transition zone and establishment of a biogeochemical reaction network for dissimilatory nitrate reduction. 2.) Determining the thermodynamic properties of Fe-phyllosilicates and their capacity and rates for electron exchange. 3.) Elucidating the enzymology of native bacteria facilitating iron reduction and oxidation. 4.) Formulating a pore-scale model of the transition zone to simulate the complex coupling of microbiologic, biogeochemical, and diffusive transport processes controlling elemental fluxes and speciation states.

Next Steps: Continued MLS sampling of the targeted wells through March 2014 will provide a robust and unique data set defining biogeochemical processes and fluxes associated with the regionally important redox transition zone over a complete yearly hydrologic cycle. Genomic analyses will be applied to DNA extracted from the sand pack samples to determine the community structure above and below the transition zone, and whether it varies on a seasonal basis as the velocity, direction, and composition of groundwater change. Of particular interest will be whether methane-oxidizing organisms are noted above the transition zone, and whether their spatial distribution correlates with methane fluxes and the known distribution of deeper zones of high organic matter localization.

Future research will develop and exercise an extended biogeochemical reactive transport model for the redox transition zone to understand its influence on the larger GWSWIZ in which it is embedded. The model domain will include highly transmissive, oxidized sediments above, and reduced sediments and carbon sources below. The biogeochemical reaction networks in the model will be informed and constrained by: i.) the above mentioned genomics analyses, and ii.) laboratory characterization and thermodynamic modeling of electron donors and acceptors. Initial model parameterization will be based on laboratory reactive diffusion and transport experiments, with subsequent assimilation and calibration to the robust MLS data set from the field. Iterations between these parameter sets will provide insights on scale dependencies and emergent behaviors to motivate additional research.

<u>Expected Contributions</u>: The Hanford-Ringold contact and the associated redox transition zone is a regional feature within the unconfined aquifer along the Columbia River shoreline. Our initial measurements on this zone suggest that it is a major source of methane to overlying groundwaters, and potentially to the Columbia River as well. This experiment will provide new insights on the existent microbial community, the process interactions that lead to the creation and maintenance of this zone, and the biogeochemical reaction rates and fluxes of C, N, S, and Fe within it. Ancient carbon is the likely driver of this system, and measurements performed within this activity will define turnover rates for buried organic carbon within the lower Columbia River Basin and the potential magnitude of methane fluxes that result. A multi-component biogeochemical transport model will be a research product that may be used to simulate the influence of this zone on C, N, and nutrient dynamics within the larger Columbia River GWSWIZ.

Publication Venues

SFA investigators published in the following journals during the reporting period that spans calendar years 2012-2013 (note **Appendix A** for citations). Our scientific impact has been large over an impressive disciplinary space, and addressing a range of spatial and temporal scales. Journal impact factors are noted in parentheses.

Acta Crystallographica Section F – Structural Biology and Crystallization Communications, Advances in Water Resources (2.412), American Mineralogist (2.026), Applied and Environmental Microbiology (3.778), Biochemical Journal (5.016), Biochemical Society Transactions (3.989), Bio Techniques (2.399), Biophysical Journal (3.668), Environmental Microbiology (5.756), Environmental Science and Technology (5.257), Frontiers in Microbiology, Geochimica et Cosmochimica Acta (4.101), Geophysics (1.723), ISME Journal (8.951), Journal of the American Chemical Society (9.023), Journal of Biological Chemistry (5.328), Journal of Colloid and Interface Science (3.172), Journal of Contaminant Hydrology (2.885), Journal of Petroleum and Environmental Biotechnology (new), Journal of Physical Chemistry C (4.814), Journal of Physical Chemistry Letters (6.585), Journal of the American

Chemical Society (10.677), Langmuir (4.187), mBio (5.621) Molecular Microbiology (4.961), Physical Chemistry Chemical Physics (3.829), Proceedings of the National Academy of Sciences (USA, 9.737), Radiochimica Acta (1.373), Structure (5.994), Vadose Zone Journal (2.200), Water Research (4.655), and Water Resources Research (3.149).

Future Scientific Vision and Goals

The PNNL SFA team is establishing a new vision for future research that aligns with the CESD Strategic Plan and revised scope of the SBR program. The PNNL SFA has provided two briefings to BER/SBR in September 2012 and April 2013 on our evolving research plans for FY2014 and beyond. More detailed scientific plans for the remainder of FY 2013 and 2014 were given in posters presented at the annual SBR P.I. meeting in May 2013 and in last year's annual report (July 2012). Research over the next term (July 2013-2014) will complete the two large multi-investigator field experiments on river water intrusion and the redox transition zone described previously, including associated laboratory experimentation to parameterize process models, and multi-process modeling of hydrologically driven biogeochemical fluxes in the GWSWIZ. The SFA-developed, linked hydrogeophysics code will also be finalized and rigorously tested against field data.

An enhanced emphasis has been placed on genomics and metagenomics (note new hire W. Nelson, **Appendix C**) in the SFA to quantify ecological drivers of community structure and inform potential metabolic pathways driving subsurface biogeochemical processes. To this end, a user proposal "Subsurface Microbial Community Function and Ecology of the Hanford Reach Groundwater-River Interaction Zone," was submitted by the PNNL microbiology team to the 2013 JGI Community Sequencing Program. The request for 2 Tb of total sequence is to enable large-scale sequencing of GWSWIZ field samples to capture spatiotemporal environmental structure. An objective of the new SFA science plan, if the CSP is supported, will be to advance the general understanding of how environmental transitions influence the functioning of ecosystems.

The SFA team is developing a new 3-year research plan for FY2015 to FY2017 to be delivered to BER in February 2014 for peer review. An internal workshop will occur in July 2013 to refine future research directions and scope, and to identify sub-teams and their leads to develop new integrated research concepts, write science plan sections, and conduct the research. Our current vision is to retain focus on understanding the GWSWIZ and developing multi-scale models for the elemental biogeochemistry of the Columbia River surface water – groundwater interaction zone with increased emphasis on larger scales. New research will focus on understanding how coupled hydrological, microbiological, and geochemical processes in the GWSWIZ influence fluxes of C and N at local and regional scales while providing new insights on GWSWIZ processes that may regulate the future discharge of Hanford contaminants to the Columbia River (e.g., ^{129}I, ^{99}Tc, and NO_3^-). Science plan details are subject to change as results accrue from our two ongoing system scale studies along the Columbia River GWSWIZ.

One option being considered for local and regional scale subsurface biogeochemical research during FY2015-2017 is to evaluate how GWSWIZ processes including heterotrophic and autotrophic respiration, methanogenesis and CH_4 oxidation, and gas evasion (e.g., CO_2, N_2O)

influence Columbia River C and N budgets. Research would involve modeling, multi-location sampling and analysis campaigns within and beyond the Hanford Site, and process specific studies at our established 300 Area field site. Observational measurements would extend to multiple locations in the Columbia River Basin. For modeling, the CLM-PFLOTRAN (under development by project P.I. Hammond) or another suitable CESD community model would be modified to include the: i.) hydrogeologic and ecosystem structures, and ii.) genomics-informed biogeochemical process interactions and dynamics of the Columbia River GWSWIZ quantified through our FY2012-2014 research. This new code would facilitate additional hypothesis formulation, and enable transparent modeling of the influence of SWGWIZ processes on carbon-nitrogen dynamics within the Columbia River system at multiple scales leading to that considered in earth system models. The overall research goal would be to quantify GWSWIZ processes and modify regional land models for improved calculations of CO_2, CH_4, and N_2O fluxes from watersheds and large surface water bodies. This research option would enable the vertical integration of the PNNL-SBR SFA with CESD-funded earth system modeling activities at PNNL.

New Scientific Research that May Shift Focus

None to report.

Collaborative Research

The PNNL SFA maintains a modest program of collaborative research. These collaborators have worked closely with PNNL research teams; complementing expertise, enriching research results, and enhancing impact (note co-authors in SFA publications, **Appendix A**). Funding provided to external collaborators (**Section V.**) has supported graduate students and post-docs, and enabled specialized analyses beyond the expertise of PNNL staff. Current collaborators, their expertise, and theme area of contribution are noted immediately below.

J. Blumberger (*University College of London*) – Electron transfer modeling, Theme Area III
D. Richardson (*University of East Anglia*) – Molecular microbiology, Theme Area III
E. Roden (*University of Wisconsin*) – Bacterial N, Fe, and S cycling, Theme Area II

V. Staffing and Budget Summary

Information is provided below on the distribution of SFA funding to PNNL staff and external collaborators in FY 2013. Below we report funding allocations for SFA Management, Theme Area I, Theme Area II, Theme Area III, and external collaborators. We also note post-docs and other post-graduate student appointees associated with Theme Area Research. The FY 2013 budget allocation from BER was $5,133,500.

Dollars from 2012 were carried over to 2013 in preparation for a difficult budgetary year. These funds included $266,704 from the IFRC project and $428,179 from the SFA. An accounting of the carry-over funds is not given below. This funding was used primarily for publications (IFRC), well-field instrumentation and staffing to support the river water intrusion study, and waste disposal. We expect minimal carryover from FY 2013 to FY 2014.

Funding Allocation by Program Element and Individual Researcher

SBR SFA Management

NAME	FTE's	FY13 BUDGET
Zachara,John M	0.49	
Fredrickson,Jim K	0.30	
Geffen, Charlette		
Other Labor	0.76	
Total	**1.55**	**616,546**

Theme Area I: Complex System Analysis and Multi-Scale Models

NAME	FTE's	FY13 BUDGET
Chen, Xingyuan	0.60	
Hammond, Glenn	0.33	
Murray, Chris	0.19	
Liu, Chongxuan	0.65	
Post Doctorate	1.01	
Other Labor	0.57	
Total	**3.35**	**914,500**

Theme Area I - Post Doc / Masters / Post Bac		
NAME	**FTE's**	**Student Type**
Shang,Jianying ***	0.98	Post Doctorate
Parker, Kyle R	0.03	Masters Intern
Total	**1.01**	

Theme Area II: Field Experiments in the GWRIZ

NAME	FTE's	FY13 BUDGET
Konopka, Allan	0.13	
McKinley, Jim	0.24	
Fredrickson, Jim	0.04	
Johnson, Tim *	0.37	
Wilkins, Mike	0.37	
Stegen, James **		
Post Doctorate	0.54	
Other Labor	2.17	
Total	**3.86**	**1,316,357**

Theme Area II - Post Doc / Masters / Post Bac		
NAME	**FTE's**	**Student Type**
Gartman,Brandy N	0.06	Post Masters
Lund,Rachael M	0.37	Post Masters
Parker, Kyle R	0.11	Masters Intern
Total	**0.54**	

Theme Area III: Functional Analyses and Process Models

NAME	FTE's	FY13 BUDGET
Rosso, Kevin	0.16	
Shi, Liang	0.41	
Felmy, Andy	0.30	
Nelson, William	0.46	
Scheibe, Tim	0.13	
Zachara, John	0.13	
Post Doctorate	2.35	
Other Labor	2.63	
Total	**6.57**	**1,982,675**

Theme Area III - Post Doc / Masters / Post Bac		
NAME	**FTE's**	**Student Type**
Chatman, Shawn M	0.09	Post Doctorate
Liu,Yimo	1.00	Post Doctorate
Shi,Zhi ***	0.23	Post Doctorate
Singh,Abhas ***	0.97	Post Doctorate
Other	0.06	Post Doctorate
Total	**2.35**	

Waste Disposal

NAME	FTE's	FY13 BUDGET
Tom Resch	0.18	
Other Labor	0.01	
Total	**0.19**	**148,246**

External Collaborators

NAME	FTE's	FY13 BUDGET
Richardson UEA		152,285
Roden UW		142,250
Blumberger UCL		21,141
Other Labor	0.05	9,000
Total		**324,676**

* Tim Johnson is funded from carryover
** James Stegen - Linus Pauling Felllowship
*** Post Doctorate assignments are complete

Personnel Actions and Procedures

Dr. William Nelson from the Wrigley Marine Science Center of the University of Southern California was hired at the beginning of FY 2013 (**Appendix C**). His expertise is in the analysis of microbial genomics emphasizing bioinformatics. He has well integrated into the SFA research team and his recent meta-genomics analyses of 300 A groundwater micro-organisms are providing important and fascinating new insights on the diversities of microbial functions in our oligotrophic system with microenvironments and transition zones. Dr. Nelson is participating in our SFA research team that is working to conceptualize and develop a new biogeochemical reactive transport model that integrates molecular information on microbial ecology and community function with geochemical reaction and hydrologic transport.

Two of our recent new hires on the SFA have left the lab during FY 2013. One was for personal reasons (Mike Wilkins) and the other was because of changing SFA research scope (Carolyn Pearce).

The SBR-SFA, in concert with a BSSD-FSFA on microbial interactions, has recently made a job offer to Dr. James Stegen who has been an EMSL Linus Pauling Distinguished Postdoctoral Fellow working with Dr. Allan Konopka (SFA P.I.) for the past two years (**Appendix C**). James completed his PhD at the University of Arizona in 2009 in Ecology and Evolution. James has been working with the SFA project team on the microbial ecology of the 300 A subsurface system on his post-doctoral research, and he will expand this role as a full time staff member beginning in January 2014. Dr. Stegen has developed a unique ecological modeling approach that the SFA plans to integrate with biogeochemical reaction network models and hydrologic transport.

Contingent on funding, the SBR-SFA is considering a new hire, or new PNNL project participant, in FY 2014 with expertise in modeling carbon biogeochemistry from the pedon to watershed scale, and knowledge of earth system models. The individual would join our modeling team (Theme Area 1), contribute to the development of an integrated SBR watershed model (with other lab SBR SFA's), and function as an interface (bridging scales) between PNNL SBR-SFA researchers and the CESD-supported earth system modeling team at PNNL.

We continue to reduce our post-doctoral count, while honoring contractual agreements, to allow re-staffing in response to scope changes in the SBR program. Two post-docs working with Dr. Zachara on Theme Area III research, for example, have recently completed their assignments and found full time positions elsewhere. Funds that covered these two positions in FY2013 will be directed towards a new-hire with climate related expertise in FY 2014 such as that described in the preceding paragraph.

The PNNL SBR-SFA has also been collaborating with Dr. Nancy Hess in her development of new, improved methods for dissolved and particulate organic matter characterization in EMSL. These methods (FTCIR-MS specifically) are being applied to field samples from our FY 2013 Columbia River Intrusion and Redox Transition Zone field campaigns. In this manner Dr. Hess has been functioning as a SFA staff member, a situation that we may formalize in FY 2014.

National Lab Investments in Program

None to report.

Appendix A: SFA Journal Publications

2013

Alexandrov V. and Rosso K. M. (2013) First-principles insights into the mechanism of Fe(II) adsorption and oxidation at Fe-clay mineral surfaces. *Journal of Physical Chemistry Letters*, Submitted.

Alexandrov V., Neumann A., Scherer M. M., and Rosso K. M. (2013) Electron exchange and conduction in nontronite from first-principles. *The Journal of Physical Chemistry C* 117, (5) 2032-2040.

Batuk O. N., Conradson S. D., Boukhalfa H., Burakov B. E., Clark D. L., Czerwinski K. R., Felmy A. R., Lezama-Pacheco J. S., Kalmykov S. N., Moore D. A., Myasoedov B. F., Reilly D. D., Roback R. C., Vlasova I. E., Webb S. M., and Wilkerson M. P. (2013) Environmental and forensic chemistry of U and Pu at Chernobyl, McGuire AFB, Mayak, Rocky Flats, Hanford, and Los Alamos. *Energy & Environmental Science*, Submitted.

Buck E. C., Felmy A. R., Moore D. A., and Czerwinski K. R. (2013) Nature of nano-sized plutonium particles in soils at the Hanford Site. *Radiochimica Acta*, In Press.

Chen X., Hammond G. E., Murray C., Rockhold M., Vermeul V. R., and Zachara J. M. (2013) Applications of ensemble-based data assimilation techniques for aquifer characterization using tracer data at Hanford 300 Area. *Water Resources Research*, Accepted.

Felmy A. R., Moore D. A., Qafoku O., Buck E. C., Conradson S. D., and Ilton E. S. (2013) Heterogeneous reduction of $^{239}PuO_2$ by aqueous Fe(II) in the presence of hematite. *Radiochimica Acta*, In Press.

Fonseca B. M., Tien M., Rivera M., Shi L., and Louro R. O. (2013) Efficient and selective isotopic labeling of hemes to facilitate the study of multiheme proteins. *Bio Techniques*, In Press.

Hammond G. E., Lichtner P. C., and Mills R. T. (2013) Evaluating the performance of parallel subsurface simulators: An illustrative example with PFLOTRAN. *Water Resources Research*, Submitted.

Kerisit S. and Liu C. (2013) Aqueous uranyl(VI) cation: Structure, kinetics, and thermodynamics from an atomistic potential model. *Physical Chemistry Chemical Physics*, Submitted.

Latta D. E., Pearce C. I., Rosso K. M., Kemner K. M., and Boyanov M. I. (2013) Reaction of UVI with titanium-substituted magnetite: Influence of Ti on UIV speciation. *Environmental Science & Technology* 47, (9) 4121-4130.

Lee J. H., Zachara J. M., Fredrickson J. K., Heald S. M., McKinley J. P., Plymale A. E., Resch C. T., and Moore D. A. (2013) Fe(II)- and sulfide-facilitated reduction of $^{99}Tc(VII)O_4^-$ in microbially reduced hyporheic zone sediments. *Geochimica et Cosmochimica Acta*, In Revision.

Liu C., Shang J., Kerisit S., Zachara J. M., and Zhu W. (2013) Scale-dependent rates of uranyl surface complexation reaction in sediments. *Geochimica et Cosmochimica Acta* 105, (0) 326-341.

Liu J., Pearce C. I., Liu C., Wang Z., Shi L., Arenholz E., and Rosso K. M. (2013) $Fe_{3-x}Ti_xO_4$ nanoparticles as tunable probes of microbial metal oxidation. *Journal of the American Chemical Society*, DOI: 10.1021/ja4015343.

Ma R., Liu C., Greskowiak J., Prommer H., Zheng C., and Zachara J. (2013) Influence of calcite on uranium(VI) reactive transport in the groundwater-river mixing zone. *Journal of Contaminant Hydrology*, Submitted.

Ma R., Zheng C., and Liu C. (2013) Groundwater impacts of radioactive wastes and associated environmental modeling assessment. In, *Encyclopedia of Sustainability Science and Technology*. In Press. Meyers, R. A. (Ed.), Springer.

Ma R., Zheng C., Liu C., Greskowiak J., Prommer H., and Zachara J. (2013) Assessment of controlling processes for field-scale uranium reactive transport under highly transient flow conditions. *Water Resources Research*, Submitted.

McKinley J. P., Zachara J. M., Resch C. T., Lund R. M., Vermeul V. R., Miller M. D., Fritz B. G., Chen X., and Murray C. J. (2013) River stage influences on the unconfined aquifer and contaminant uranium fluxes adjacent to the Columbia River on the Hanford Site, Washington. *Water Resources Research*, Submitted.

McMillan D. G., Marritt S. J., Judd E. T., Shi L., Richardson D. J., Evans S. D., Elliott S. J., Butt J. N., and Jeuken L. J. (2013) Protein-protein interaction regulates the direction of catalysis and electron transfer in a redox enzyme complex. *Journal of the American Chemical Society*, In Revision.

Murray C. J., Zachara J. M., McKinley J. P., Ward A., Bott Y.-J., Draper K., and Moore D. (2013) Establishing a geochemical heterogeneity model for a contaminated vadose zone – aquifer system. *Journal of Contaminant Hydrology*, (http://dx.doi.org/10.1016/j.jconhyd.2012.02.003)

Over M. W., Yang Y., Chen X., and Rubin Y. (2013) Making Bayesian inversion efficient using singular value decomposition and clustering. *Water Resources Research*, Submitted.

Pearce C. I., Liu J., Baer D. R., Qafoku O., Heald S., Arenholz E., Grosz A. E., Mckinley J. P., Resch C. T., Bowden M. E., Engelhard M. H., and Rosso K. M. (2013) Characterization of natural titanomagnetites ($Fe_{3-x}Ti_xO_4$) for studying heterogeneous electron transfer to Tc(VII) in the Hanford subsurface. *Geochimica et Cosmochimica Acta*, Submitted.

Renslow R. S., Babauta J. T., Dohnalkova A., Boyanov M. I., Kemner K. M., Majors P. D., Fredrickson J. K., and Beyenal H. (2013) Metabolic spatial variability in electrode-respiring Geobacter sulfurreducens biofilms. *Energy & Environmental Science*, In Press.

Richmond M. C., Perkins W. A., Scheibe T. D., Lambert A., and Wood B. D. (2013) Flow and axial dispersion in a sinusoidal-walled tube: Effects of inertial and unsteady flows. *Advances in Water Resources*, Submitted.

Scheibe T. D., Hou Z., and Palmer B. J. (2013) Pore-scale simulation of intragranular diffusion: Effects of incomplete mixing on macroscopic manifestations. *Water Resources Research*, In Press.

Shang J. Y., Liu C., Wang Z., and Zachara J. M. (2013) Long-term kinetics of U(VI) desorption from sediments. *Water Resources Research*, Submitted.

Shelobolina E., Benzine J., Xiong M. Y., and Roden E. (2013) Microbial agents of phyllosilicate-Fe redox cycling in Hanford 300 sediments. *Frontiers in Microbiology*, Submitted.

Smith D. M. A. and Rosso K. M. (2013) Molecular dynamics of decaheme cytochrome MtrF of S. oneidensis suggests possible conformationally-gated electron transport mechanism. *Biophysical Journal*, Submitted.

Stegen J. C., Lin X., Fredrickson J. K., Chen X., Kennedy D. W., Murray C., Rockhold M., and Konopka A. (2013) Quantifying community assembly processes and identifying features that impose them. *ISME Journal*, In Press.

Stoliker D. L., Liu C., Kent D. B., and Zachara J. M. (2013) Characterizing particle-scale equilibrium adsorption and kinetics of uranium(VI) desorption from U-contaminated sediments. *Water Resources Research* 49, 1-15, doi:10.1002/wrcr.20104.

Sycheva L. V., Eggleston C. M., Magnuson T. S., Colberg P. J. S., Adam N., Zhang H. Z., Johnson P., and Shi L. (2013) Redox-linked conformation changes in adsorbed c-type cytochromes from *Shewanella oneidensis* MR-1 adsorbed to oxide surfaces. *Langmuir*, In Review.

Wallin E. L., Johnson T. C., Greenwood W. J., and Zachara J. M. (2013) Imaging high stage river-water intrusion into a contaminated aquifer along a major river corridor using 2-D time-lapse surface electrical resistivity tomography. *Water Resources Research* 49, 1-16.

White G. F., Shi Z., Shi L., Wang Z., Dohnalkova A. C., Marshall M. J., Fredrickson J. K., Zachara J. M., Butt J. N., Richardson D. J., and Clarke T. A. (2013) Rapid electron exchange between surface-exposed bacterial cytochromes and Fe(III) minerals. *Proceedings of the National Academy of Sciences* 110, (16) 6346-6351.

Wilkins M. J., Kennedy D. W., Castelle C. S., Field E. K., Stepanauskas R., Fredrickson J. K., and Konopka A. (2013) Single-cell genomics reveal metabolic strategies for growth and survival in the Hanford 300 Area aquifer. *mBio*, Submitted.

Yang X., Scheibe T. D., Richmond M. C., Perkins W. A., Vogt S. J., Codd S. L., Seymour J. D., and McKinley M. I. (2013) Direct numerical simulation of pore-scale flow in a bead pack:

Comparison with magnetic resonance imaging observations. *Advances in Water Resources* 54, (0) 228-241.

Zachara J. M., Long P. E., Bargar J., Davis J. A., Fox P., Fredrickson J. K., Freshley M. D., Konopka A. E., Liu C., McKinley J. P., Rockhold M. L., Williams K. H., and Yabusaki S. B. (2013) Persistence of uranium groundwater plumes: Contrasting mechanisms at two DOE sites in the groundwater–river interaction zone. *Journal of Contaminant Hydrology* 147, (0) 45-72.

Zachara J. M., Ilton E. S., and Liu C. (2013) Reactive transport of the uranyl ion in soils, sediments, and groundwater systems. In, *Uranium - Cradle to Grave*. 255-300. Burns, P. C. and Sigmon, G. E. Eds. Published by the Mineralogical Association of Canada (MAC), Québec, Canada.

Zhang C., Liu C., and Shi Z. (2013) Micromodel investigation of transport effect on the kinetics of reductive dissolution of hematite. *Environmental Science & Technology* 47, (9) 4131-4139.

Zhang X., Liu C., Hu B. X., and Zhang G. (2013) Uncertainty analysis of multi-rate kinetics of uranium desorption. *Journal of Contaminant Hydrology*, Submitted.

2012

Ahmed B., Cao B., McLean J. S., Ica T., Dohnalkova A., Istanbullu O., Paksoy A., Fredrickson J. K., and Beyenal H. (2012) Fe(III) Reduction and U(VI) immobilization by Paenibacillus sp strain 300A, isolated from Hanford 300A subsurface sediments. *Applied and Environmental Microbiology* 78, (22) 8001-8009.

Ahmed B., Cao B., Mishra B., Boyanov M. I., Kemner K. M., Fredrickson J. K., and Beyenal H. (2012) Immobilization of U(VI) from oxic groundwater by Hanford 300 Area sediments and effects of Columbia River water. *Water Research* 46, (13) 3989-3998.

Breuer M., Zarzycki P., Blumberger J., and Rosso K. M. (2012) Thermodynamics of electron flow in the bacterial deca-heme cytochrome MtrF. *Journal of the American Chemical Society* 134, (24) 9868-9871.

Breuer M., Zarzycki P., Shi L., Clarke T. A., Edwards M. J., Butt J. N., Richardson D. J., Fredrickson J. K., Zachara J. M., Blumberger J., and Rosso K. M. (2012) Molecular structure and free energy landscape for electron transport in the decahaem cytochrome MtrF. *Biochemical Society Transactions* 40, (6) 1198-1203.

Cao B., Majors P. D., Ahmed B., Renslow R. S., Silvia C. P., Shi L., Kjelleberg S., Fredrickson J. K., and Beyenal H. (2012) Biofilm shows spatially stratified metabolic responses to contaminant exposure. *Environmental Microbiology* 14, (11) 2901-2910.

Chen X. Y., Murakami H., Hahn M. S., Hammond G. E., Rockhold M. L., Zachara J. M., and Rubin Y. (2012) Three-dimensional Bayesian geostatistical aquifer characterization at the Hanford 300 Area using tracer test data. *Water Resources Research* 48.

Edwards M. J., Fredrickson J. K., Zachara J. M., Richardson D. J., and Clarke T. A. (2012) Analysis of structural MtrC models based on homology with the crystal structure of MtrF. *Biochemical Society Transactions* 40, (6) 1181-1185.

Edwards M. J., Hall A., Shi L., Fredrickson J. K., Zachara J. M., Butt J. N., Richardson D. J., and Clarke T. A. (2012) The crystal structure of the extracellular 11-heme cytochrome UndA reveals a conserved 10-heme motif and defined binding site for soluble iron chelates. *Structure* 20, (7) 1275-1284.

Ewing R. P., Liu C. X., and Hu Q. H. (2012) Modeling intragranular diffusion in low-connectivity granular media. *Water Resources Research* 48.

Felmy A. R., Moore D. A., Pearce C. I., Conradson S. D., Qafoku O., Buck E. C., Rosso K. M., and Ilton E. S. (2012) Controls on soluble Pu concentrations in PuO_2/magnetite suspensions. *Environmental Science & Technology* 46, (21) 11610-11617.

Ilton E. S., Wang Z. M., Boily J. F., Qafoku O., Rosso K. M., and Smith S. C. (2012) The effect of pH and time on the extractability and speciation of uranium(VI) sorbed to SiO_2. *Environmental Science & Technology* 46, (12) 6604-6611.

Johnson T. C., Versteeg R. J., Rockhold M., Slater L. D., Ntarlagiannis D., Greenwood W. J., and Zachara J. (2012) Characterization of a contaminated wellfield using 3D electrical resistivity tomography implemented with geostatistical, discontinuous boundary, and known conductivity constraints. *Geophysics* 77, (6) EN85-EN96.

Kerisit S. and Liu C. X. (2012) Diffusion and adsorption of uranyl carbonate species in nanosized mineral fractures. *Environmental Science & Technology* 46, (3) 1632-1640.

Konopka A. and Wilkins M. (2012) Application of meta-transcriptomics and -proteomics to analysis of *in situ* physiological state. *Frontiers in Microbiology* 3.

Lee J. H., Fredrickson J. K., Kukkadapu R. K., Boyanov M. I., Kemner K. M., Lin X. J., Kennedy D. W., Bjornstad B. N., Konopka A. E., Moore D. A., Resch C. T., and Phillips J. L. (2012) Microbial reductive transformation of phyllosilicate Fe(III) and U(VI) in Fluvial subsurface sediments. *Environmental Science & Technology* 46, (7) 3721-3730.

Lichtner P. C. and Hammond G. E. (2012) Using high performance computing to understand roles of labile and nonlabile uranium(VI) on Hanford 300 Area plume longevity. *Vadose Zone Journal* 11, (2).

Lilova K. I., Pearce C. I., Gorski C., Rosso K. M., and Navrotsky A. (2012) Thermodynamics of the magnetite-ulvospinel (Fe_3O_4-Fe_2TiO_4) solid solution. *American Mineralogist* 97, (8-9) 1330-1338.

Lilova K. I., Xu F., Rosso K. M., Pearce C. I., Kamali S., and Navrotsky A. (2012) Oxide melt solution calorimetry of Fe^{2+}-bearing oxides and application to the magnetite-maghemite (Fe_3O_4-$Fe_{8/3}O_4$) system. *American Mineralogist* 97, (1) 164-175.

Lin X. J., Kennedy D., Peacock A., McKinley J., Resch C. T., Fredrickson J., and Konopka A. (2012) Distribution of microbial biomass and potential for anaerobic respiration in Hanford Site 300 Area subsurface sediment. *Applied and Environmental Microbiology* 78, (3) 759-767.

Lin X. J., McKinley J., Resch C. T., Kaluzny R., Lauber C. L., Fredrickson J., Knight R., and Konopka A. (2012) Spatial and temporal dynamics of the microbial community in the Hanford unconfined aquifer. *ISME Journal* 6, (9) 1665-1676.

Lin X., Kennedy D., Fredrickson J., Bjornstad B., and Konopka A. (2012) Vertical stratification of subsurface microbial community composition across geological formations at the Hanford Site. *Environmental Microbiology* 14, (2) 414-425.

Liu C. and Fang Y. (2012) Kinetic modeling of microbiological processes. *Journal of Petroleum & Environmental Biotechnology* 3:e109.

Liu J., Pearce C. I., Qafoku O., Arenholz E., Heald S. M., and Rosso K. M. (2012) Tc(VII) reduction kinetics by titanomagnetite ($Fe_{3-x}Ti_xO_4$) nanoparticles. *Geochimica et Cosmochimica Acta* 92, 67-81.

Liu J., Wang Z., Belchik S. M., Edwards M. J., Liu C., Kennedy D. W., Merkley E. D., Lipton M. S., Butt J. N., Richardson D. J., Zachara J. M., Fredrickson J. K., Rosso K. M., and Shi L. (2012) Identification and characterization of MtoA: A decaheme c-Type cytochrome of the neutrophilic Fe(II)-oxidizing bacterium sideroxydans lithotrophicus ES-1. *Frontiers in Microbiology* 3.

Ma R., Zheng C. M., Zachara J. M., and Tonkin M. (2012) Utility of bromide and heat tracers for aquifer characterization affected by highly transient flow conditions. *Water Resources Research* 48.

Marritt S. J., Lowe T. G., Bye J., McMillan D. G., Shi L., Fredrickson J., Zachara J., Richardson D. J., Cheesman M. R., Jeuken L. J., and Butt J. N. (2012) A functional description of CymA, an electron-transfer hub supporting anaerobic respiratory flexibility in *Shewanella*. *Biochemical Journal* 444, (3) 465-474.

Marritt S. J., McMillan D. G., Shi L., Fredrickson J. K., Zachara J. M., Richardson D. J., Jeuken L. J., and Butt J. N. (2012) The roles of CymA in support of the respiratory flexibility of *Shewanella oneidensis* MR-1. *Biochemical Society Transactions* 40, (6) 1217-1221.

Nguyen H. D., Cao B., Mishra B., Boyanou M. I., Kemner K. M., Fredrickson J. K., and Beyenal H. (2012) Microscale geochemical gradients in Hanford 300 Area sediment biofilms and influence of uranium. *Water Research* 46, (1) 227-234.

Pearce C. I., Qafoku O., Liu J., Arenholz E., Heald S. M., Kukkadapu R. K., Gorski C. A., Henderson C. M. B., and Rosso K. M. (2012) Synthesis and properties of titanomagnetite ($Fe_{3-x}Ti_xO_4$) nanoparticles: A tunable solid-state Fe(II/III) redox system. *Journal of Colloid and Interface Science* 387, 24-38.

Pearce C. I., Wilkins M. J., Zhang C. Y., Heald S. M., Fredrickson J. K., and Zachara J. M. (2012) Pore-scale characterization of biogeochemical controls on iron and uranium speciation under flow conditions. *Environmental Science & Technology* 46, (15) 7992-8000.

Peng S., Hu Q. H., Ewing R. P., Liu C. X., and Zachara J. M. (2012) Quantitative 3-D elemental mapping by LA-ICP-MS of a basaltic clast from the Hanford 300 Area, Washington, USA. *Environmental Science & Technology* 46, (4) 2025-2032.

Peretyazhko T. S., Zachara J. M., Kukkadapu R. K., Heald S. M., Kutnyakov I. V., Resch C. T., Arey B. W., Wang C. M., Kovarik L., Phillips J. L., and Moore D. A. (2012) Pertechnetate (TcO_4^-) reduction by reactive ferrous iron forms in naturally anoxic, redox transition zone sediments from the Hanford Site, USA. *Geochimica et Cosmochimica Acta* 92, 48-66.

Plymale A. E., Bailey V. L., Fredrickson J. K., Heald S. M., Buck E. C., Shi L., Wang Z. M., Resch C. T., Moore D. A., and Bolton H. (2012) Biotic and abiotic reduction and solubilization of $Pu(IV)O_2 \bullet xH_2O_{(am)}$ as affected by anthraquinone-2,6-disulfonate (AQDS) and ethylenediaminetetraacetate (EDTA). *Environmental Science & Technology* 46, (4) 2132-2140.

Richardson D. J., Butt J. N., Fredrickson J. K., Zachara J. M., Shi L., Edwards M. J., White G., Baiden N., Gates A. J., Marritt S. J., and Clarke T. A. (2012) The 'porin-cytochrome' model for microbe-to-mineral electron transfer. *Molecular Microbiology* 85, (2) 201-212.

Richardson D. J., Edwards M. J., White G. F., Baiden N., Hartshorne R. S., Fredrickson J., Shi L., Zachara J. M., Gates A. J., Butt J. N., and Clarke T. A. (2012) Exploring the biochemistry at the extracellular redox frontier of bacterial mineral Fe(III) respiration. *Biochemical Society Transactions* 40, (3) 493-500.

Richardson D. J., Fredrickson J. K., and Zachara J. M. (2012) Electron transport at the microbe-mineral interface: A synthesis of current research challenges. *Biochemical Society Transactions* 40, (6) 1163-1166.

Roden E. E. (2012) Microbial iron-redox cycling in subsurface environments. *Biochemical Society Transactions* 40, 1249-1256.

Roden E., McBeth J. M., Blöthe M., Percak-Dennett E. M., Fleming E. J., Holyoke R. R., Luther G. W., and Emerson D. (2012) The microbial ferrous wheel in a neutral pH groundwater seep. *Frontiers in Microbiology* 3.

Shelobolina E. S., Konishi H., Xu H., Benzine J., Xiong M. Y., Wu T., Blöthe M., and Roden E. (2012) Isolation of phyllosilicate-iron redox cycling microorganisms from an illite-smectite rich hydromorphic soil. *Frontiers in Microbiology* 3.

Shelobolina E., Xu H. F., Konishi H., Kukkadapu R., Wu T., Blothe M., and Roden E. (2012) Microbial lithotrophic oxidation of structural Fe(II) in biotite. *Applied and Environmental Microbiology* 78, (16) 5746-5752.

Shi L., Rosso K. M., Clarke T. A., Richardson D. J., Zachara J. M., and Fredrickson J. K. (2012) Molecular underpinnings of Fe(III) oxide reduction by *Shewanella oneidensis* MR-1. *Frontiers in Microbiology* 3.

Shi L., Rosso K. M., Zachara J. M., and Fredrickson J. K. (2012) Mtr extracellular electron-transfer pathways in Fe(III)-reducing or Fe(II)-oxidizing bacteria: A genomic perspective. *Biochemical Society Transactions* 40, (6) 1261-1267.

Shi Z., Zachara J. M., Shi L., Wang Z. M., Moore D. A., Kennedy D. W., and Fredrickson J. K. (2012) Redox reactions of reduced flavin mononucleotide (FMN), riboflavin (RBF), and anthraquinone-2,6-disulfonate (AQDS) with ferrihydrite and lepidocrocite. *Environmental Science & Technology* 46, (21) 11644-11652.

Singer D. M., Chatman S. M., Ilton E. S., Rosso K. M., Banfield J. F., and Waychunas G. A. (2012) Identification of simultaneous U(VI) sorption complexes and U(IV) nanoprecipitates on the magnetite (111) surface. *Environmental Science & Technology* 46, (7) 3811-3820.

Singer D. M., Chatman S. M., Ilton E. S., Rosso K. M., Banfield J. F., and Waychunas G. A. (2012) U(VI) sorption and reduction kinetics on the magnetite (111) surface. *Environmental Science & Technology* 46, (7) 3821-3830.

Stegen J. C., Lin X. J., Konopka A. E., and Fredrickson J. K. (2012) Stochastic and deterministic assembly processes in subsurface microbial communities. *ISME Journal* 6, (9) 1653-1664.

Tomanicek S. J., Johs A., Sawhney M. S., Shi L., and Liang L. (2012) Crystallization and preliminary X-ray crystallographic studies of the outer membrane cytochrome OmcA from *Shewanella oneidensis* MR-1. *Acta Crystallographica Section F-Structural Biology and Crystallization Communications* 68, 53-55.

Wang Y., Sevinc P. C., Belchik S. M., Fredrickson J., Shi L., and Lu H. P. (2012) Single-cell imaging and spectroscopic analyses of Cr(VI) reduction on the surface of bacterial cells. *Langmuir* 29, (3) 950-956.

White G. F., Shi Z., Shi L., Dohnalkova A. C., Fredrickson J. K., Zachara J. M., Butt J. N., Richardson D. J., and Clarke T. A. (2012) Development of a proteoliposome model to probe transmembrane electron-transfer reactions. *Biochemical Society Transactions* 40, (6) 1257-1260.

Appendix B: SFA Presentations

2013

Chen X., Hammond G. E., Vermeul V. R., and Zachara J. M. (2013) "Improving the Reactive Transport Modeling at the Hanford 300 Area with a Bayesian Data Assimilation Framework." Presented by Xingyuan Chen, Glenn Hammond, Vince Vermeul, John Zachara (Invited Speaker) at DOE BER SBR/TES Joint Investigator Meeting 2013, Potomac, MD on May 14, 2013. PNNL-SA-95584.

Fredrickson J. K. (2013) "Environmental Biogeochemistry of ^{99}Technetium: Implications for Subsurface Transport at the Hanford Site." Presented by James K. Fredrickson (Invited Speaker) at 4th Annual Patricia Durbin Memorial Lecture at LBNL, Berkeley, CA on May 29, 2013. PNNL-SA-95932.

Johnson T. C., Chen X., and Hammond G. E. (2013) "System Scale Imaging and Modeling of Groundwater-River Water Exchange at the Hanford 300 Area." Presented by Tim Johnson, Glenn Hammond, Xingyuan Chen (Invited Speaker) at DOE SBR/TES Joint Investigator Meeting, on May 14, 2013. PNNL-SA-95568.

Liu C., Zachara J. M., Shang J., Zhang C., Kerisit S. N., Zhang X., and Hu B. X. (2013) "Development of Multi-Scale Process Models for Complex Subsurface Systems." Presented by Chongxuan Liu at SBR/TES Joint Investigator Meeting, Potomac, MD on May 16, 2013. PNNL-SA-95775.

McKinley J. P., Murray C. J., Chen X., Resch C. T., Miller M. D., Lund R. M., and Zachara J. M. (2013) "Using Dynamic Groundwater U Concentrations to Infer the Impacts of Couples Processes in a Complex, Heterogeneous Subsurface Environment." Presented by John M. Zachara at SBR/TES Joint Investigator Meeting, Potomac, MD on May 14, 2013. PNNL-SA-95692.

Nelson W. C., Konopka A., Wilkins M. J., and Stegen J. C. (2013) "Effect of Groundwater-River Exchange on Microbial Community Structure and Function." Presented by William C. Nelson at 2013 TES/SBR Joint Investigator Meeting, Potomac, MD on May 13, 2013. PNNL-SA-95564.

Rosso K. M., Pearce C. I., Liu J., Qafoku O., Shi L., Alexandrov V. Y., Smith D. M. A., Felmy A. R., Neumann A., Scherer M., Breuer M., Blumberger J., and Arenholz E. (2013) "Redox Behavior of 300 A Fe-Phyllosillicates, Fe-Oxides and Key Biomolecules." Presented by Kevin M. Rosso (Invited Speaker) at 2013 SBR/TES Joint Investigator Meeting, Potomac, MD on May 14, 2013. PNNL-SA-95716.

Shang J. (2013) "Multiple-scale Investigation of Particle and Contaminant Transport in Critical Zone." Presented by Jianying Shang (Invited Speaker) at Virginia Polytechnic Institute and State University, Blacksburg, VA on May 31, 2013. PNNL-SA-95821.

Shi L., Liu Y., Kennedy D. W., Shi Z., Wang Z., Dohnalkova A., Roden E. E., Levar C. C., Bond D. R., White G. F., Richardson D. J., Konopka A., Rosso K. M., Zachara J. M., and Fredrickson J. K. (2013) "Electron Transfer Mechanisms for Microbial Iron Redox Cycle in Hanford Subsurface Sediments." Presented by Liang Shi at 2013 SBR/TES Joint Investigators Meeting, Potomac, MD on May 13, 2013. PNNL-SA-95482.

Zachara J. M., Ilton E. S., and Liu C. (2013) "Chapter 8: Reactive Transport of the Uranyl Ion in Soils, Sediments, and Groundwater Systems." Presented by John M. Zachara (Invited Speaker) at Canadian Mineralogical Society Short Course, Winnipeg, Canada on May 21, 2013. PNNL-SA-95822.

Zachara J. M., Fredrickson J. K., Konopka A., Stegen J. C., Johnson T. C., Hammond G., Wilkins M. J., Chen X., McKinley J. P., and Nelson W. C. (2013) "Investigating Biogeochemical and Microbial Community Dynamics in a Groundwater-River Water Interaction Zone Promoted by Seasonal Hydrologic Fluctuations." Presented by John M. Zachara (Invited Speaker) at SBR/TES Joint Investigator Meeting, Potomac, MD on May 15, 2013. PNNL-SA-95731.

Zachara J. M., Fredrickson J. K., McKinley J. P., Resch C. T., Miller M. D., Konopka A., Stegen J. C., Lin X., Kennedy D. W., and Wilkins M. J. (2013) "Biogeochemical Investigations Across Subsurface Oxidation-Reduction Boundaries at the Hanford Site." Presented by John M. Zachara (Invited Speaker) at SBR/TES Joint Investigator Meeting, Potomac, MD on May 15, 2013. PNNL-SA-95773.

Zachara J. M., Shi Z., Fredrickson J. K., Shi L., Wang Z., White G. F., and Richardson D. (2013) "Electron Transfer Between Micro-Organisms and Mineral Phases: Unraveling the Mechanism and Thermodynamic, Kinetic, and Surface Chemical Controls." Presented by John M. Zachara (Invited Speaker) at 12th International Conference on the Biogeochemistry of Trace Elements, Athens, GA on June 18, 2013. PNNL-SA-96470.

Zachara J. M. (2013) "Environmental Geochemistry of Uranium in a Coupled Vadose Zone-Groundwater-River System." Presented by John M. Zachara (Invited Speaker) at Washington State University, Richland, WA on April 10, 2013. PNNL-SA-94913.

<u>2012</u>

Hammond G. E., and Chen X. (2012) "Data Assimilation at the Hanford 300 Area." Presented by Glenn E. Hammond, Xingyuan Chen (Invited Speaker) at 2012 GSA Annual Meeting and Exposition, Charlotte, NC on November 4, 2012. PNNL-SA-89809.

Kerisit S. N., Felmy A. R., and Liu C. (2012) "Molecular Simulations of Diffusion and Adsorption Processes in Nano-Sized Mineral Fractures." Presented by Sebastien N. Kerisit (Invited Speaker) at BES-Geosciences Workshop: Reaction and Transport Within Internal Domains of Porous Media, San Francisco, CA on December 1, 2012. PNNL-SA-92280.

Liu C., Zachara J. M., Shang J., and Zhang C. (2012) "Synergetic Coupling of Intragranular Reactions and Transport." Presented by Chongxuan Liu (Invited Speaker) at DOE BES Workshop, San Francisco, CA on December 2, 2012. PNNL-SA-92418.

Lykens K. E., Alderson P. A., and Shi L. (2012) "Cytochrome Purification from Fe (III)-Reducing *Shewanella oneidensis*." Presented by Kimberly E. Lykens at The Wittenberg University Noyce Fall Colloquium, Springfield, OH on September 18, 2012. PNNL-SA-89687.

Rosso K. M. (2012) "Frontiers in Molecular Biogeochemistry: Electron Transfer Dynamics in the Redox Cycling of Iron." Presented by Kevin M. Rosso (Invited Speaker) at Invited Smith Lecture at the University of Michigan Department of Earth and Environmental Sciences, Ann Arbor, MI on October 26, 2012. PNNL-SA-91951.

Shang J., Liu C., Varga T., and Zachara J. M. (2012) "Pore-Scale Exploration of Uranyl Transport and X-ray CT Geological Applications." Presented by Jianying Shang (Invited Speaker) Beijing, China on July 10, 2012. PNNL-SA-89151.

Zachara J. M., Fredrickson J. K., Chen X., Felmy A. R., Hammond G. E., Konopka A., Liu C., McKinley J. P., Murray C. J., Pearce C. I., Richardson D., Roden E. E., Rosso K. M., Scheibe T. D., Shi L., and Wilkins M. J. (2012) "SBR SFA Transition Plan: Hydrobiogeochemical Process Dynamics in the Groundwater-River Interaction Zone." Presented by John Zachara and Jim Fredrickson (Invited Speaker) at Briefing to SBR, Richland, WA on September 12, 2012. PNNL-SA-90632.

Zachara J. M. (2012) "Multi-Scale Mass Transfer Processes Controlling Biogeochemistry and Reactive Transport in a Groundwater-River Interaction Zone." Presented by John M. Zachara (Invited Speaker) at Interagency Steering Committee on Multimedia Environmental Models (ISCMEM) Annual Meeting, Reston, VA on November 7, 2012. PNNL-SA-91953.

Zhu Z., Wang Z., Zachara J. M., and Singh A. (2012) "ToF-SIMS and NanoSIMS Imaging of Uranium Distributions in the Sediment of Hanford 300 Area." Presented by Zihua Zhu at 22nd International Conference on the Application of Accelerators in Research and Industry, Fort Worth, TX on August 10, 2012. PNNL-SA-90175.

Appendix C: New Staff

William Cheesman Nelson
Pacific Northwest National Laboratory
902 Battelle Blvd; PO Box 999, MSIN J4-19
Richland, WA 99352
Email: william.nelson@pnnl.gov; Phone: 509-375-4442

Education

National Institute of Allergy and Infectious Disease, Laboratory of Viral Disease
IRTA Fellow 1996-1998

University of North Carolina at Chapel Hill, Dept of Biology
Ph.D. in Biology, May 1996
Honors: University Merit Assistantship, 1990-91, University Graduate Travel Grant, 1994.

Bucknell University
BAs in Biology and Chemistry, June 1990
Honors: Diamond State Scholarship, 1986-90, elected into Phi Sigma 1989

Professional Appointments

Sep 2012 – present, Scientist, Pacific Northwest National Laboratory, Biological Sciences Division

May 2007 – Aug 2012, Research Assistant Professor, University of Southern California, Dana and David Dornsife College of Letter, Arts & Sciences, Department of Biological Sciences, Marine Environmental Biology Section

Oct 2004 – Apr 2007, Bioinformatics Analyst Manager, The Institute for Genomic Research, Microbial Annotation team

Oct 1998 – Sept 2004, Bioinformatics Analyst, The Institute for Genomic Research, Microbial Annotation team

Professional Affiliations

American Association for the Advancement of Science
American Society of Microbiology

Research Interests

Genome sequencing technologies allow us to gather data about microbes without the need to culture them. This allows us to explore what mechanisms they use to survive under the wide variety of environmental conditions in which they are found. The vast quantities of data generated require special expertise to handle. I have a great deal of experience processing and analyzing microbial genomic information. I want to apply my skills and the new sequencing technologies and bioinformatics techniques to the development of microbial solutions to energy and pollution problems.

Selected Publications

1. Nelson WC, Bhaya D, Heidelberg JF. (2012) Novel miniature transposable elements in thermophilic Synechococcus strains and their impact on an environmental population. *J Bacteriol.* 194(14):3636-42.
2. Koid A, Nelson WC, Mraz A, Heidelberg KB. (2012) Comparative analysis of eukaryotic marine microbial assemblages from 18S rRNA gene and gene transcript clone libraries by using different methods of extraction. *Appl Environ Microbiol.* 78(11):3958-65.
3. Tully BJ, Nelson WC, Heidelberg JF. (2011) Metagenomic analysis of a complex marine planktonic thaumarchaeal community from the Gulf of Maine. *Environ Microbiol*. 2011 Nov 3. [Epub ahead of print]
4. Biddle JF, Sylvan JB, Brazelton WJ, Tully BJ, Edwards KJ, Moyer CL, Heidelberg JF, Nelson WC.(2011) Prospects for the study of evolution in the deep biosphere. *Front Microbiol*. 2011; 2:285.
5. Nelson WC, Bhaya D, Heidelberg JF. (2011) Analysis of Insertion Sequences in Thermophilic Cyanobacteria: Exploring the Mechanisms of Establishing, Maintaining, and Withstanding High Insertion Sequence Abundance. *Appl Environ Microbiol* 77(15).
6. Singer E, Emerson D, Webb EA, Barco RA, Kuenen JG, Nelson WC, Chan CS, Comolli LR, Ferriera S, Johnson J, Heidelberg JF, Edwards KJ. (2011) Mariprofundus ferrooxydans PV-1 the first genome of a marine Fe(II) oxidizing Zetaproteobacterium. *PLoS One*. 6(9):e25386. Epub 2011 Sep 23.
7. Singer E, Webb EA, Nelson WC, Heidelberg JF, Ivanova N, Pati A, Edwards KJ. (2011) Genomic Potential of *Marinobacter aquaeolei*, a biogeochemical "opportunitroph". *Appl Environ Microbiol*. 77(8):2763-71.
8. Ward NL, Challacombe JF, Janssen PH, Henrissat B, Coutinho PM, Wu M, Xie G, Haft DH, Sait M, Badger J, Barabote RD, Bradley B, Brettin TS, Brinkac LM, Bruce D, Creasy T, Daugherty SC, Davidsen TM, Deboy RT, Detter JC, Dodson RJ, Durkin AS, Ganapathy A, Gwinn-Giglio M, Han CS, Khouri H, Kiss H, Kothari SP, Madupu R, Nelson K, Nelson WC, Paulsen I, Penn K, Ren Q, Rosovitz MJ, Selengut JD, Shrivastava S, Sullivan SA, Tapia R, Thompson LS, Watkins KL, Yang Q, Yu C, Zafar N, Zhou L, Kuske CR. (2009) Three genomes from the phylum Acidobacteria provide insight into their lifestyles in soils. *Appl Environ Microbiol.* 2009 Apr; 75(7):2046-56. Epub 2009 Feb 5.
9. Venter JC, Remington K, Heidelberg JF, Halpern AL, Rusch D, Eisen JA, Wu D, Paulsen I, Nelson KE, Nelson W, Fouts DE, Levy S, Knap AH, Lomas MW, Nealson K, White O, Peterson J, Hoffman J, Parsons R, Baden-Tillson H, Pfannkoch C, Rogers YH, Smith HO. (2004) Environmental genome shotgun sequencing of the Sargasso Sea. *Science*. 304(5667):66-74.
10. Beja O, Suzuki MT, Heidelberg JF, Nelson WC, Preston CM, Hamada T, Eisen JA, Fraser CM, DeLong EF. (2002) Unsuspected diversity among marine aerobic anoxygenic phototrophs. *Nature* 415(6872): 630-633.

James C. Stegen
Linus Pauling Distinguished Postdoctoral Fellow
Pacific Northwest National Laboratory
Microbiology Group, Biological Sciences Division
902 Battelle Boulevard, P.O. Box 999, MSIN J4-18, Richland, WA 99352
Email: James.Stegen@pnnl.gov; Phone: 509-371-6763; Fax: 509-371-6955
Website: http://www.pnl.gov/science/staff/staff_info.asp?staff_num=7731

Education

Central Washington University	Biology	B.A. 2000
Eastern Washington University	Biology	M.S. 2004
University of Arizona	Ecology & Evolution	Ph.D. 2009
University of North Carolina	Biology	Postdoc 2009-2011
Pacific Northwest National Laboratory	Microbiology	Postdoc 2011-present

Research Interests

Dr. Stegen works to merge theoretical and empirical approaches within spatial ecology in order to understand the processes that govern the composition of ecological communities and the functioning of ecosystems. His current research further combines multiple 'omics' approaches with the statistical and conceptual foundations of spatial ecology to better understand microbial communities and their dynamic linkages to geochemistry and hydrology.

Scientific and Academic Appointments

2011-present. Linus Pauling Fellow (Pacific Northwest National Laboratory)
2009-2011. NSF Postdoctoral Fellow in bioinformatics (Allen Hurlbert, faculty sponsor)
2007-2009. Research Associate (NSF-FIBR): University of Arizona (P.I., Regis Ferriere)
2005. Field Research Associate at RMBL: University of Arizona (P.I., Brian Enquist)
2004-2007. Teaching Associate: University of Arizona
2001-2004. Teaching Assistant: Eastern Washington University
2002-2004. Biological survey of Banks Lake: Subcontracted via WA State Fish & Wildlife
2001-2003. Biological survey of northeast WA lakes: Subcontracted via Kalispell Tribe
2001. Columbia River salmon survey: Subcontracted via Pacific Northwest National Lab
2001. Yakima River salmon/trout survey: Subcontracted via WA State Fish & Wildlife
2000. Effect of UV radiation on alpine tadpoles: Univ. of WA research field assistant

Publications

1. Stegen, J.C., et al. Estimating and mapping community assembly processes in the subsurface. *Ecology*, in review.
2. Stegen, J.C., et al. 2013. Quantifying community assembly processes and identifying features that impose them. *ISME Journal*, in press.
3. Wang, J., J. Shen, Y. Wu, T. Chen, J. Soininen, J.C. Stegen, et al. 2013. Phylogenetic beta-diversity in bacterial communities across ecosystems: deterministic vs. stochastic processes. *ISME Journal*, in press.
4. Bentley, L.P., J.C. Stegen, et al. 2013. An empirical assessment of metabolic scaling theory using branch-level and whole-tree external branching patterns. *Ecology Letters*, in press.

5. Bailey, V.L., S.J. Fansler, J.C. Stegen, and L.A. McCue. 2013. Linking microbial community structure to β-Glucosidic function in soil aggregates. *ISME Journal*, in press.
6. Stegen, J.C., et al. 2013. Stochastic and deterministic drivers of spatial and temporal turnover in breeding bird communities. *Global Ecology and Biogeography*, 22:202-212.
7. Moles, A.T., B. Peco, I.R. Wallis, W.J. Foley, A.G.B. Poore, A.J. Bisigato, L. Cella-Pizarro, C.J. Clark, P.S. Cohen, W.K. Cornwell, W. Edwards, R. Ejrnaes, T. Gonzales-Ojeda, B.J. Graae, G. Hay, F.C. Lumbwe, B. Magaña-Rodríguez, B.D. Moore, P.L. Peri, J.R. Poulsen, J.C. Stegen, et al. 2013. Correlations between physical and chemical defenses in plants: Trade-offs, syndromes, or just many different ways to skin a herbivorous cat? *New Phytologist*, 198:252-263.
8. Stegen, J.C., X. Lin, A.E. Konopka, and J.K. Fredrickson. 2012. Stochastic and deterministic assembly processes in subsurface microbial communities. *ISME Journal*, 6:1653-64.
9. Price, C.A., J.S. Weitz, V.M. Savage, J.C. Stegen, A. Clarke, D. A. Coomes, P.S. Dodds, R.S. Etienne, A.J. Kerkhoff, K. McCulloh, K.J. Niklas, H. Olff and N.G. Swenson. 2012. Testing the metabolic theory of ecology. *Ecology Letters*, 15:1465-1474.
10. Kraft, N.J.B., N.J. Sanders, J.C. Stegen, et al. 2012. Response to comments on "disentangling the drivers of β diversity along latitudinal and elevational gradients". *Science* 335:1573.
11. Stegen, J.C., R. Ferriere, and B.J. Enquist. 2012. Eco-evolutionary community dynamics: covariation between richness and invasibility across temperature gradients. *American Naturalist*, 180: E110-126.
12. Hulshof, C.M., J.C. Stegen, N.G. Swenson, C.A.F. Enquist, and B.J. Enquist. 2012. Interannual variability of growth and reproduction in the tropical tree *Bursera simaruba*: The role of allometric size dependency and climatic variability. *Ecology*, 93: 180-190.
13. Swenson, N.G., B.J. Enquist, J. Pither, A.J. Kerkhoff, B. Boyle, M.D. Weiser, J.J. Elser, W.F. Fagan, J. Forero-Montaña, N. Fyllas, N.J.B. Kraft, J.K. Lake, A.T. Moles, S. Patiño, O.L. Phillips, C. A. Price, P.B. Reich, C.A. Quesada, J.C. Stegen, et al. 2012. The biogeography and filtering of woody plant functional diversity in North and South America. *Global Ecology and Biogeography*, 21: 798-808.
14. Stegen, J.C., R. Ferriere, and B.J. Enquist. 2012. Evolving ecological networks and the emergence of biodiversity patterns across temperature gradients. *Proceedings of the Royal Society B: Biological Sciences* 279:1051-1060.
15. McClain, C.R., J.C. Stegen, and A.H. Hurlbert. 2012. Dispersal, environmental niches and oceanic-scale turnover in deep-sea bivalves. *Proceedings of the Royal Society B: Biological Sciences*, 279: 1993-2002.
16. Swenson, N.G., J.C. Stegen, et al. 2012. Temporal turnover in the composition of tropical tree communities: functional determinism and phylogenetic stochasticity. *Ecology*, 93: 490-9.
17. Kraft, N.J.B., L.S. Comita, J.M. Chase, N.J. Sanders, N.G. Swenson, T.O. Crist, J.C. Stegen, et al. 2011. Disentangling the drivers of β diversity along latitudinal and elevational gradients. *Science* 333:1755-1758. **Science cover article*
18. Moles, A.T., I.R. Wallis, W.J. Foley, D.I. Warton, J.C. Stegen, et al. 2011. Putting plant resistance traits on the map: a test of the idea that plants are better defended at lower latitudes. *New Phytologist* 191:777-788.
19. Stegen, J.C. and A.R. Black. 2011. Trophic ecology of an aquatic mite (*Piona carnea*) preying on Daphnia pulex: effects of predator density, nutrient supply and a second predator (*Chaoborus americanus*). *Hydrobiologia* 668:171-182.