Environmental System Science

Summary of projects awarded in summer 2020 under the Environmental System Science Funding Opportunity Announcement DE-FOA-0002184.

Program Overview

The goal of the Environmental System Science (ESS) activity in the U.S. Department of Energy's Office of Science, Office of Biological and Environmental Research (BER) is to advance a robust predictive understanding of terrestrial environments, extending from bedrock to the top of the vegetated canopy and from molecular to global scales in support of DOE's energy and environmental missions. Using an iterative approach to model-driven experimentation and observation, inter-disciplinary teams of scientists work to unravel the coupled physical, chemical and biological processes that control the structure and functioning of terrestrial ecosystems and watershed systems across vast spatial and temporal scales. State-of-science understanding is captured in conceptual theories and models which can be translated into a hierarchy of computational components and used to predict the system response to perturbations caused, for example, by changes in climate, land use/cover or contaminant loading. Basic understanding of the system structure and function is advanced through this iterative cycle of experimentation and observation by targeting key system components and processes that are suspected to most limit the predictive skill of the models. The ESS activity is comprised of the Terrestrial Ecosystem Science (TES) and the Subsurface Biogeochemical Research (SBR) programs.

Funding Opportunity Announcement Overview

The Funding Opportunity Announcement (FOA) DE-FOA-0002184, was issued by the Environmental System Science program and released in the Fall of 2019. The goal of this FOA was to improve the understanding and representation of terrestrial ecosystem and subsurface environmental processes in ways that advance the sophistication and capabilities of local, regional, and larger scale models (e.g., Energy Exascale Earth System Model, E3SM). Using new measurements, field experiments, more sophisticated modeling and/or synthesis studies, this FOA encompassed two topic areas: 1) Terrestrial Ecology, and 2) Subsurface and Watershed Hydro-biogeochemistry.

Applications to this FOA were expected to take a systems approach to understand ecosystems and watershed functioning over the multiple temporal and spatial scales that are represented in models (e.g., single process models, ecosystem or watershed models, and global models). This emphasis on the capture of advanced empirical and theoretical understanding in models had two goals. First, it sought to improve the representation of these integrated processes in coupled models, thereby increasing the sophistication of the projections. Second, it encouraged the community to understand and use a diversity of existing models and to compare model results against observations or other data sets to identify knowledge gaps and future research directions. It also sought to encourage an iterative dialog between the empirical and modeling research communities such that research objectives were co-designed to address key model deficiencies and that modeling efforts were designed to inform empirical research. By connecting the modeling and experimental components, this approach maximizes the return on scientific investments by reducing duplication of efforts and encourages collaboration, thus generating a significant benefit to both the Department of Energy and the scientific community. Research in Environmental System Science also provides a public benefit through experiments, observations and modeling that acts to inform next-generation model projections of ecosystem processes, watershed function, and disturbances that can be used in decision support.

Overall, the FOA considered research applications that included and coupled measurements, experiments, modeling or synthesis to provide improved quantitative and predictive understanding of terrestrial ecosystems and watershed function spanning the continuum from the bedrock through vegetation to the atmospheric interface. All projects were required to clearly delineate an integrative, hypothesis-driven approach and clearly describe the existing needs/gaps in state-of-the-art models. Applicants were required to provide details on how the results of the proposed research, if successful, would be incorporated into appropriate scale models and model frameworks. While the TES and SBR programs support a broad spectrum of fundamental research in environmental system science and considered research applications within this scope, this FOA particularly encouraged applications in the following Science Areas:

<u>TES Science Area 1 – Interactions and Feedbacks between Above- and Belowground Processes</u>: Improved understanding of the interactions and feedbacks among key above- and below-ground ecological and biogeochemical components/processes that span the functional soil-microbe-plant-atmosphere continuum, that in turn enables robust process-level understanding and improved Earth system projections across scales.

Applications that examine coupled biogeochemical cycles, system thresholds, and/or factors that create and sustain biogeochemical "hot spots" and "hot moments" were particularly encouraged. While applications were not required to target all components of the soil-microbe-plant-atmosphere continuum, successful applications must have clearly identified targeted aboveground and belowground processes and the specific interactions between these components and or processes.

<u>TES Science Area 2 – Ecological Controls and Feedbacks on the Methane Cycle</u>: New or improved understanding of the ecological controls on methane fluxes, particularly those related to hot spot-hot moment phenomena that have the potential for direct feedbacks to the Earth system.

Successful applications were required to include the collection of new CH_4 measurements in order to expand the limited, but growing CH_4 datasets for future synthesis, model development and analysis. Applications that examined factors that created, sustained and/or limited hot spot-hot moment phenomena for CH_4 fluxes were particularly encouraged, as well as those that leveraged the AmeriFlux network's "Year of Methane" where appropriate.

<u>SBR Science Area 3 – Existing Watersheds:</u> Hydro-biogeochemistry, biogeochemistry and geochemistry research to advance understanding of watershed function at existing watershed testbeds.

Successful applications were required to compliment SBR Science Focus Area research activities at current SBR watershed testbed sites, by exploring new directions to address identified science gaps at a particular existing testbed. Emphasis was placed on reaction- and watershed-scale modeling applications, including catchment microbiology and watershed vegetation, and on river basin and regional-scale modeling applications focused on hydrologic processes and prediction, particularly for water/mass balances and evapotranspiration. These applications were required to discuss approaches for validating model outputs/results with field- or lab-based experimentation.

SBR Science Area 4 – Novel Watersheds: Hydro-biogeochemistry, biogeochemistry and geochemistry research to study the functioning of watershed structural components that are novel to the SBR program.

Successful applications were required to focus on important structural components of watersheds that are not present in the current SBR testbeds: headwater springs; gaining and/or losing streambeds (other than those associated with the SFAs); and tidal and/or freshwater mouths of watersheds. This science area sought applications that investigated the hydro-biogeochemical functioning of these missing natural components of integrated watershed systems in the continental U.S. only. Additionally, efforts were required to describe whether or not the proposed research had the potential to become, or would become, a part of the WHONDRS network.

Overall, proposed research was intended to fill critical knowledge gaps, including the exploration of high-risk approaches. BER encouraged the submission of innovative riskier, exploratory applications with potential for future high impact on TES and SBR research.

Nine awards (three of which were exploratory awards) were made through this Funding Opportunity Announcement totaling $6,097,609 over three years.

Funded Projects

Terrestrial Ecosystem Science (TES) Awards

Functional-Type Modeling Approach and Data-Driven Parameterization of Methane Emissions in Wetlands

- **Principle Investigators:** Gil Bohrer (Ohio State University) and Eric Ward (U.S. Geological Survey)
- **Collaborators:** Kelly Wrighton (Colorado State University); Jorge Vila (University of Louisiana at Lafayette), William Riley (Lawrence Berkeley National Laboratory)
- **Total Award:** $999,779 over 3 years
- **Award Type:** Standard

The role of natural wetland emissions in the recent sharp increase of global methane atmospheric concentration is hotly debated. Difficulties in modeling methane emissions are driven, to a large degree, by the spatially heterogeneous nature of wetland ecosystems and by the high temporal and spatial variability of methane fluxes. This variability in fluxes is a result of the underlying heterogeneity of the wetlands, combined with the complex and interconnected belowground and aboveground processes of methane production, consumption, and transport. Eddy covariance (EC) and chamber flux measurements, and remote sensing of wetlands and atmospheric methane concentrations are routinely used to parameterize and improve land-surface models that predict methane fluxes. However, model optimizations are typically done against observations of the net site-level flux, or coarse atmospheric methane concentration and do not independently address within-wetland heterogeneity or the various processes that add up to the net flux. Therefore, even models that make accurate CH_4 emission predictions may be right for the wrong reasons.

The goal of this project is to improve simulation of methane emissions from coastal wetlands in the E3SM Land Model (ELM). We will improve

ELM along three spatial and conceptual axes: (i) Patch resolution – expand the subgrid surface-tile approach, currently widely utilized in representation of upland vegetation, to represent ecohydrological patch types, such as open-water, mudflats, emergent/floating vegetation, swap forest, etc. (ii) Vertical resolution – provide vertically detailed observations of belowground dissolved methane concentration gradients and utilize ELMs patch-level vertical soil column to resolve methane production, oxidation, and transport at high vertical resolution. (iii) Process resolution– increasing the number, type, and accuracy of independent process representations that combine within the soil column and interact with plants to affect net CH_4 emissions.

To support these model developments, we propose to expand an already extensive dataset of observations in 4 coastal wetlands along salinity and tidal influence gradient. Observations include flux measurements at multiple scales: whole-site EC fluxes (in 3 sites, already reporting to AmeriFlux), chamber flux measurements at each ecohydrological patch type, bubble accumulations, and methane transport through plants. These measurements will allow us to directly test and parameterize the model at multiple scales, including specific processes resolved at the patch level, and go beyond the typical whole-site parameterization. Observations also include vertical profiles of methane, dissolved organic carbon, oxygen, and temperature in the soil of each patch type, using in-situ dialysis samplers (peepers). Soil cores for chemistry, metagenomic and meta-transcriptomics, and methane, and carbon isotope analysis, will provide estimates of the presence and relative importance of the rates of particular microbial processes of production and consumption of methane. We will conduct sets of parameterization, validation, and sensitivity analyses simulations using the PEcAn workflow. After the optimization of the model at our demonstration site, we will use the framework of the Global Carbon Project methane reanalysis simulations to test the sensitivity of global methane emission forecasts to resolving sub-site ecohydrological patches.

Our project will significantly improve ELM coastal-wetland methane simulation capabilities by implementing the sub-site ecohydrological patch-type approach, improving process representation, and careful testing and calibration against multi-scale observations. We will demonstrate the process-level multi-scale parameterization approach and provide direct observations to determine and directly constrain parameters within the multiple methane biogeochemical and plant processes represented in ELM. We will demonstrate the need for global within-wetland patch characterization and delineation, and patch-level flux and vertically detailed concentration observations.

Sticky Roots — Implications of Altered Rhizodeposition (Driven by Cryptic, Viral Infection of Plants) for the Fate of Rhizosphere Mineral–Organic Matter Associations in Natural Ecosystems

- **Principle Investigator:** Zoe Cardon (Marine Biological Laboratory))
- **Collaborators:** Marco Keiluweit (University of Massachusetts); Carolyn Malmstrom (Michigan State University), William Riley (Lawrence Berkeley National Laboratory)
- **Total Award:** $999,244 over 3 years
- **Award Type:** Standard

Mineral-associated organic matter (MAOM) is a dominant component of total soil carbon, and once bound to reactive soil minerals, organic matter (OM) can be protected from enzymatic attack for millennia. We are striving to understand mechanisms by which plant roots can dislodge OM from soil minerals, making it available to enzymatic attack and/or biological uptake. Model compounds common in rhizodeposits can destabilize MAOM in laboratory assays, spurring its mineralization by microbes and soil carbon loss, and, potentially, pulling associated nutrients into actively cycling pools. The importance of MAOM in belowground biogeochemistry has therefore spurred ongoing development in DOE's ELM model (the land model within the new Energy Exascale Earth System Model). If rhizodeposition has the power to mobilize MAOM, the vast reservoir of OM bound to minerals must be viewed as accessible, at a cost, to plants and the soil microbial community in an abiotic–biotic commodities exchange.

A major challenge in this project is that our target belowground driver–rhizodeposition–is dynamic and largely invisible in soils of natural ecosystems. A novel twist of the planned work therefore lies in the aboveground treatment through which we will perturb belowground function: controlled viral infection. Overall phloem flow is increased by virus infection, potentially spurring increased delivery of phloem contents to growing root tips and the surrounding rhizosphere, making them "sticky." Virus infection also often decreases root to shoot ratio, meaning that shoot demands for nutrients must be met by more intensive mining of soil per unit root.

We plan an intensive greenhouse experiment explicitly to test whether the presence of plant roots drives mobilization and mineralization of MAOM, and whether the extent of mobilization and mineralization shifts as a function of differential rhizodeposition. We also will delve more deeply into mechanisms underlying how plant roots interact with and mobilize MAOM, at the scale of single roots and whole root systems, using functionally diverse grasses (C3 and C4, annual and perennial, fine-rooted and coarse-rooted, virus-infected and uninfected). Process-level understanding derived from these data will inform development and sensitivity testing of an improved representation of dynamic OM-mineral associations in ELM, incorporating vulnerability to rhizodeposition, potentially with notable implications for long-term soil carbon storage and nutrient availability.

We will test four hypotheses:

H1. Rhizodeposition leads to mobilization and mineralization of MAOM.

H2. Altered rhizodeposition per unit root, driven by viral infection, increases mobilization of MAOM (per unit root biomass).

H3. Decreased plant root biomass and root system spatial reach (e.g. as driven by viral infection) reduces whole-soil-column mobilization and mineralization of MAOM.

H4. In ELM simulations, root-driven mobilization will transiently reduce existing MAOM pools, but ultimately will increase overall soil carbon stocks.

Our linked experimental and modeling efforts are responsive to this FOA in that we are examining a major uncertainty associated with controls over biogeochemical cycling of one of the largest stable terrestrial C pools in temperate and tropical soils – mineral-associated OM. And if viral infection does consistently lead to "sticky roots", our perception of the potential importance of prevalent virus infection for the terrestrial carbon cycle will be transformed.

Remote Sensing of Plant Functional Traits for Modeling Arctic Tundra Carbon Dynamics

- **Principle Investigator:** Jennifer Fraterrigo (University of Illinois)
- **Collaborators:** Eugenie Euskirchen (University of Alaska, Fairbanks); Shawn Serbin (Brookhaven National Laboratory)
- **Total Award:** $998,745 over 3 years
- **Award Type:** Standard

Permafrost carbon feedbacks to global climate are a major concern because the Arctic is warming twice as fast as other regions and >50% of the global belowground organic carbon (C) pool is stored in permafrost and overlying soils. Thawing of permafrost and frozen soils can expose organic C to decomposition, potentially converting these ecosystems into sources of CO_2 and accelerating warming. Plant communities in the Arctic tundra are also responding to warming, and these changes are expected to alter key biogeochemical and physical processes that feedback to climate. However, the direction and magnitude of effects are highly uncertain because tundra vegetation responses to warming are non-uniform and poorly represented in models.

The proposed research develops capacity for the remote estimation of aboveground and belowground plant functional traits and streamlines their inclusion in process models to quantify and predict regional C balance. Specifically, we will characterize directly observable plant functional traits from remotely sensed data; predict non-observable (e.g., belowground) traits by leveraging trait-environment relationships and trait covariation; and integrate this information into a newly developed modeling framework to quantify and predict terrestrial C stocks, fluxes, and their uncertainties in the Alaskan tundra. We will test four hypotheses: (1) Plant functional traits are predominantly shaped by climate, with local soil moisture moderating trait response to climate, but optimal trait values for a given environment depend on community type because plant functional types (PFTs) have different sensitivities to altered resources associated with climate warming. (2) Trait dispersion depends on environmental stress; where environmental conditions are more favorable for growth, there is greater variation in traits and overall greater trait diversity; (3) Given trait tradeoffs and trait-environment interactions, root traits are predictable from leaf and size traits, climate and soil factors; and (4) Variation in traits affect Arctic C balance. Leaf traits as they relate to photosynthetic parameters will have the strongest effects on C uptake. Root traits will exhibit fewer direct effects on C uptake but will be important in supporting nutrient uptake that then influences C uptake. To test these hypotheses, we will study the variation in plant traits across the major tundra vegetation communities present along local soil gradients nested within a macroclimate gradient in northern Alaska, quantifying trait-environment relationships and trait covariation at the community- and PFT-levels. Using machine-learning approaches, we will integrate ground-based measurements with information derived from multi-scale remote sensing platforms from drone, hypertemporal, LiDAR, and hyperspectral imagery to produce maps of leaf, size and root traits, greatly expanding the trait information available for modelers. We will use Bayesian data-model fusion methods to improve the parameterization and formulation of the Terrestrial Ecosystem Model, which is widely used in Arctic carbon studies, and perform simulation experiments to evaluate how differences in plant functional traits affect C dynamics. To synergize the trait-based modeling community, we will create a workshop to share findings and strategies for improving the representation of trait variation in ecosystem and Earth System Models (ESMs).

The proposed research directly supports the DOE near-term priorities by improving understanding of the interactions and feedbacks among above- and belowground plant system components and related soil-plant-atmosphere processes in a region that is inadequately represented in ESMs. Current models reduce the complexity of Arctic vegetation to a small number of PFTs. This approach implicitly assumes that each PFT represents the average ecological function of its constituent species, thus ignoring the effects of trait variation on carbon cycling and potentially leading to large uncertainty in the sign and magnitude of ecosystem feedbacks to climate. We will fill critical gaps in our understanding of the dominant PFTs and facilitate the development of alternative modeling approaches that allow the traits of PFTs to vary, thereby vastly enhancing the capacity of simulation models to project ecosystem carbon dynamics in a rapidly changing Arctic.

Understanding and Modelling Current and Future Coastal Wetland Methane

- **Principle Investigator:** Genevieve Noyce (Smithsonian Institution)
- **Collaborators:** Teri O'Meara (Smithsonian Institution), Roy Rich (Smithsonian Institution), Peter Thornton (Oak Ridge National Laboratory), Paul Brewer (Arizona State University)
- **Total Award:** $999,930 over 3 years
- **Award Type:** Standard

The coastal terrestrial-aquatic interface (TAI) is a highly dynamic component of the Earth system that plays a critical role in biogeochemical cycling. Due to its dynamic nature, the processes that regulate decomposition and methane (CH_4) emissions are of greater significance at the TAI than in upland systems. Despite this, we have limited mechanistic understanding of how climate stressors interact to regulate the electron acceptors and donors that determine decomposition pathways within TAIs, including the generation of hot spots and hot moments. Accurately modeling these processes is critical for incorporating the coastal TAI into Earth systems models, such as DOE's E3SM. With previous DOE support, we adapted an aerobic terrestrial representation of decomposition using PFLOTRAN, a reactive flow and transport model, and added anerobic decomposition pathways, salinity, and oxygen (O_2) that fluctuates independently of water table level. However, because this model ($PFLOTRAN_{TAI}$) is based on decomposition rates and organic matter carbon to nitrogen ratios from terrestrial systems, its performance in TAI systems is currently limited by the lack of empirical data to properly parameterize variables. In addition, while $PFLOTRAN_{TAI}$ can simulate movement of O_2 into sediments, it is not currently capable of tracking the movement of CH_4 gas through plant tissues due to both current model structure and lack of available data.

Our overall objective of this proposal is to improve the representation of anaerobic decomposition biogeochemistry in $PFLOTRAN_{TAI}$. Based on knowledge gaps identified during $PFLOTRAN_{TAI}$ development, we have pinpointed three specific objectives that will increase our mechanistic understanding of CH_4 dynamics in response to environmental change and improve our model representation:

Objective 1: Quantify rates of multiple anaerobic decomposition pathways that regulate CH_4 emissions, including hot moments, across varying time scales.

Objective 2: Determine the individual and interactive effects of warming, salinity, and inundation on CH_4 cycling pathways and other anaerobic decomposition processes.

Objective 3: Using an iterative process, connect field work and model development to: i) parameterize anaerobic decomposition in $PFLOTRAN_{TAI}$, focusing on CH_4 emissions, and ii) identify future areas of focus for model improvement.

We have identified the five key field measurements required to update $PFLOTRAN_{TAI}$ as: 1) relative rates of redox processes, 2) effects of global change stressors, 3) soil C quality, 4) plant-mediated transport of O_2 and CH_4, and 5) sediment heterogeneity. To accomplish this, we will integrate both field-based (natural gradient and manipulative experiments) and lab-based (redox incubations) measurements into our research plan. We propose to conduct spatial (space-for-time) monitoring at coastal sites that span a natural gradient of salinity, as well as temporal and manipulative process-level studies, looking at effects of warming, salinity, and inundation. These manipulations will include installing automated flux chambers in a novel soil heating experiment and setting up marsh organs with varying levels of warming, inundation, and salinity. Our proposed efforts will result in the collection of chamber-level CH_4 flux measurements across multiple sites, ecological conditions, and timeframes, as well as corresponding measurements on porewater chemistry, soil carbon quality, plant biomass, and redox reaction rates. Using these new datasets, we will first improve $PFLOTRAN_{TAI}$ to accurately model CH_4 emissions and then conduct sensitivity analyses to identify areas for future field studies. The updated $PFLOTRAN_{TAI}$ will be linked to the land model of E3SM and vastly improve the representation of coastal systems within a larger framework.

TES: Modelling Microbes to Predict Post-fire Carbon Cycling in the Boreal Forest across Burn Severities

- **Principle Investigator:** Thea Whitman (University of Wisconsin, Madison)
- **Collaborators:** Benjamin Sulman (Oak Ridge National Laboratory)
- **Total Award:** $299,972 over 2 years
- **Award Type:** Exploratory

Boreal forests hold between 370-1720 Pg carbon (C) above- and belowground, making them a major stock of C globally. In North American boreal ecosystems, wildfire is the primary stand-replacing disturbance, and fires are projected to increase in frequency and severity in the future. Fires have direct effects on C stocks due to immediate losses during combustion, but also have indirect effects, through the modification of soil properties and remaining soil C, the response of vegetation communities, and changes to soil microbial communities and their activities. Changes to fire frequency and severity could affect each of these processes, and changes to fire severity or frequency have, indeed, been associated with changes in soil C storage. However, data quantifying these effects are sparse, and our understanding of the mechanisms driving them remains limited.

Recent advances in Earth system model (ESM) representations of soil C cycling, such as the Carbon, Organisms, Rhizosphere and Protection in the Soil Environment (CORPSE) model, have included an emphasis on explicitly representing the system in an increasingly mechanistically accurate way. In particular, this has included: representing both physically protected and unprotected C; distinguishing between rhizosphere and bulk soil; representing microbes as dead or living, or as different functional types, among other developments. Because of their mechanistic nature, these models may be better prepared to represent the effects of wildfires on soil C dynamics than most current ESMs. Standard ESMs generally do not represent complex feedbacks between fire, vegetation, soils, microbes, and climate. Rather, they usually represent fires only in terms of their frequency and impacts on vegetation biomass pools, and predict that the above-ground community follows a well- known trajectory over time, with no new steady states other than those functionally similar to the previous state.

We propose to determine whether linking belowground microbial community composition, size, and activity to aboveground properties of burn severity and plant community composition (upland jack pine and upland spruce) allows us to better model post-fire soil CO_2 fluxes using the CORPSE model. We will use an integrated modelling-experimental approach, with mechanistic laboratory experiments designed to inform models of three hierarchical levels of complexity. Our objectives are as follows:

Objective 1. Quantify changes in C fluxes, microbial biomass, and microbial community composition, after simulated fires in intact soil cores across a burn severity gradient.

Objective 2. Develop and evaluate adaptations to the CORPSE model to better represent post-fire SOC dynamics across a burn severity gradient using data from Objective 1 across a hierarchy of model complexity: (1) no explicit microbial representation; (2) community-level microbial traits characterized by single scalable parameters – maximum growth rate, CUE, and total microbial biomass; (3) microbes characterized as an assemblage of multiple functional groups with different traits constrained by the observed experimental data across the microbial community.

Objective 3. Test the capacity of the adapted CORPSE model (Objective 2) to predict CO_2 flux rates in burned cores from new sites.

Wildfires in boreal ecosystems represent a globally significant ecological process that is expected to be sensitive to climate change, but is currently insufficiently understood and represented in models. We propose fundamental, mechanism-based and model-driven research in a globally important system with basic relevance for environmental change, addressing current modelling challenges. It will help advance understanding of Earth's biogeochemical systems and climate while developing insights into terrestrial cycling of C and nutrients, and their feedbacks with Earth's climate system, thus strengthening scientific knowledge in ecology, biology, and biogeochemistry.

Subsurface Biogeochemical Research (SBR) Awards

Quantifying Microbial Roles in Environmental Iron Oxidation via an Integrated Kinetics, 'Omics and Metabolic Modeling Study

- **Principle Investigator:** Clara Chan (University of Delaware)
- **Collaborators:** Edward O'Loughlin (Argonne National Laboratory), Pamala Weisenhorn (Argonne National Laboratory), Nancy Merino (Lawrence Livermore National Laboratory), Mavrik Zavarin (Lawrence Livermore National Laboratory), Cara Santelli (University of Minnesota), Crystal Ng (University of Minnesota)
- **Total Award:** $300,000 over 2 years
- **Award Type:** Exploratory

Iron ox(yhydrox)ides are extremely reactive components of environmental systems, and therefore exert a strong influence on biogeochemical cycles. These oxides strongly adsorb many biologically-relevant elements, including organic carbon and phosphate, as well as a wide range of metals including uranium and actinide species. Thus, the formation mechanisms of iron oxides are key to understanding both nutrient and metal contaminant cycling. Microorganisms can catalyze iron oxidation and promote the formation of iron biominerals but it is completely unknown how much of environmental iron oxidation is biologically-mediated versus abiotic. The overarching goal of our proposed work is to quantify and constrain microbial iron oxidation rates and gain insight into the controls on this process, toward an ultimate goal of integrating biotic iron oxidation into reactive transport models. The main challenge will be isolating the effects of iron oxidizing microorganisms from other competing mechanisms of iron oxidation. Therefore, the purpose of this exploratory project is to address this challenge in order to establish a clear path toward modeling environmental microbial iron oxidation.

Our work focuses on the Savannah River Site (SRS) in South Carolina, where microbial iron-oxidizers have been observed. At Tims Branch, part of the Argonne National Laboratory Wetland Hydrobiogeo-chemistry Science Focus Area (Argonne SFA), where groundwater discharges into a stream, extensive iron-oxidizing microbial mats form and appear to be a major sink of uranium. Pond B, part of the Lawrence Livermore National Laboratory (LLNL) BioGeoChemistry of Actinides SFA, is an actinide-impacted seasonally-stratified water body with iron oxidation at the chemocline, which may be due to Fe-oxidizers (based on culture evidence). Stratified ferruginous water bodies and iron mats are the most well-studied freshwater microbial iron-oxidizing systems, making the SRS an excellent field site for studying and comparing microbial iron oxidation processes in these two hydrogeochemical settings.

Our approach will combine field perturbations and measurements, kinetics experiments on iron-oxidizing mats, and metagenomics/meta-transcriptomics coupled to metabolic modeling. Our objectives are to:

1. Quantify biotic iron oxidation rates in a field setting and in iron microbial mat incubations. We will compare these rates to abiotic rates to determine the relative contributions of microbes.

2. Identify and quantify dominant iron-oxidizing microorganisms and flanking community members at both SRS sites using genome-resolved metagenomics and metatranscriptomics and integrate the results to identify trophic status and carbon utilization of dominant iron oxidizers.

3. Construct metabolic models of a well-studied iron oxidizer and the most abundant and active iron-oxidizers and flanking organisms to establish linkages between microbial iron oxidation and carbon cycling.

The collaborations between UD, Argonne and LLNL SFAs, and the University of Minnesota-led hydrogeochemistry project will allow us to take advantage of field operations, geochemical analyses, and hydrogeochemical observations from the locations that we plan to sample. Beyond these rates, a major outcome will be better protocols for obtaining reliable, replicable environmental biotic iron oxidation rates for use in modeling, and an understanding of controls on iron oxidation. We will also generate a new library of iron oxidizer metagenome-assembled genomes from both SRS sites, and by integrating with transcriptomic results, will be able to characterize the trophic status of major iron oxidizers and propose ecological linkages that connect Fe and C cycling. An additional outcome will be the first neutrophilic, iron-oxidizing bacteria metabolic model with validation (*Sideroxydans lithotrophicus* ES-1) and initial consortia-style metabolic models of iron-oxidizing communities, which will yield testable hypotheses and clear next steps for refining metabolic models for integration into watershed scale models. This work sets the stage for our longer-term goal to link iron oxidizer metabolic models and kinetics to biogeochemical/hydrological models to predict iron, carbon, nutrient and contaminant metal cycling effects.

Watershed Controls on Uranium Concentrations Tied to Natural Organic Matter in Streambeds and Wetlands

- **Principle Investigator:** Peter Santschi (Texas A&M University at Galveston)
- **Collaborators:** Daniel Kaplan (Savannah River National Laboratory), Chris Yeager (Los Alamos National Laboratory), Pamela Weisenhorn (Argonne National Laboratory), Kenneth Kemner (Argonne National Laboratory), Patrick Hatcher (Old Dominion University)
- **Total Award:** $300,000 over 2 years
- **Award Type:** Exploratory

Wetlands and their hyporheic zones, e.g., regions where groundwater and surface water exchange, display complex and seasonally-varied dynamics in hydraulic, chemical, physical and microbial properties, which result in their functioning as a sink or source of organic matter (OM) and associated contaminants, such as uranium (U). Molecular-scale understanding of the interactions between OM, U and microbes under seasonally-varied hydrological conditions (temperature, pH, Eh, water table height, rainfall, nutrient loading, etc.) in these critical zones is still not well understood, yet a full understanding of these regulating processes is crucial for the development of fundamentally sound watershed reactive transport models. Through field-oriented studies at the Argonne Wetland Hydrobiogeochemistry SFA field site (a wetland contaminated by U for over 50 years) and accompanying laboratory experiments this project seeks to 1) establish linkage of watershed hydrological conditions to U concentrations and to OM sources, abundance and composition by monitoring temporal hydrological parameters and events; 2) establish a seasonal U mass balance and flux model between solid and water bodies; 3) reveal the molecular characteristics of the organic moieties that are responsible for U binding from four types of solids that represent the major solid bodies in the wetlands and their hyporheic zones; and lastly 4) to determine relationships between the microbial community structure and gene content of wetland interfacial zones with OM properties that influence U transport. By addressing these key knowledge gaps in wetland hydro-biogeochemical processes, we will contribute to Earth System Models and help DOE advance a robust predictive understanding of how watersheds function as integrated systems and how these systems influence water quality and contaminant release.

Nutrient and Fine Sediment Transport Driven by Perturbations in River Bed Movement

- **Principle Investigator:** Elowyn Yager (University of Idaho)
- **Collaborators:** Andrew Tranmer (University of Idaho), Janice Brahney (Utah State University), Joel Rowland (Los Alamos National Laboratory)
- **Total Award:** $600,000 over 3 years
- **Award Type:** Standard

In mountainous watersheds, riverbeds are commonly composed of gravel sized sediment that undergoes episodic transport during higher magnitude flow events. Gravel-bedded rivers typically have a coarse surface layer ('armor layer') that is relatively difficult to move and protects a finer subsurface layer that is often enriched in Phosphorus (P), fine sediment, and Particulate Organic Carbon (POC). When high flow events occur, armor layer motion can release large quantities of nutrients and fines that could explain the large observed temporal variations in POC, suspended sediment (SS), and various forms of P exported from many watersheds. The relative importance of armor layer movement in controlling POC, P, and SS concentrations in rivers will vary with the streambed concentrations of these constituents. These streambed concentrations may also depend on the influence of groundwater inputs to the river reach. We test three hypotheses about armor layer motion and river concentrations of POC, P, and SS using detailed field measurements in two river reaches in the upper Jemez River basin, New Mexico. We will take high resolution measurements of armor layer movement and streambed concentrations as well as P, POC, and SS in the water column during flow events over two years. The proposed research will bring a mechanistic understanding of the linkages between geomorphology and nutrient storage, release, and transport. The study also addresses how perturbations, such as the sequence and magnitude of droughts and floods, constrain biogeochemical nutrient cycling and impact subsequent temporal variations in nutrient and fine sediment export from mountainous watersheds.

Linking Nutrient Reactivity and Transport in Subsurface Flowpaths along a Terrestrial-Estuarine Continuum

- **Principle Investigator:** Margaret Zimmer (University of California, Santa Cruz)
- **Collaborators**: Erin Seybold (Kansas Geological Survey); Anna Braswell (University of Florida), Corianne Tatariw (University of Alabama), Bhavna Arora (Lawrence Berkeley National Laboratory), Ate Visser (Lawrence Livermore National Laboratory)
- **Total Award:** $599,939 over 3 years
- **Award Type:** Standard

Salt marshes are critical "hot spots" of nutrient processing and retention and thus play an important role in improving coastal water quality. In particular, coastal salt marshes retain upwards of one-third of terrestrially derived nitrogen (N) loads, helping to mitigate negative environmental impacts such as eutrophication and harmful algal blooms. This removal is largely driven by sediment microbial activity, which is controlled by spatial and temporal variability in the availability in oxygen and organic matter. These changes in redox characteristics and substrate availability impact the pathways by which N is processed by microbes. Our study objective is to address a substantial knowledge gap in our understanding of the hydrologic and environmental factors that drive solute fate and transport at the subsurface terrestrial-marine boundary at tidal watershed mouths. At the Elkhorn Slough National Estuarine Research Reserve, we will couple field- and lab-based studies with reactive transport models to quantify the co-variation of hydrological and biogeochemical subsurface processes in coastal watersheds, with a particular emphasis on identifying drivers on N retention and removal over different hydrologic regimes. Through this effort, we are extending the DOE Scientific Focus Area testbed approach to a novel and underrepresented coastal ecosystem.

Further information on TES objectives along with a listing of past and current funding opportunities discussed in this document, is available at https://science.osti.gov/ber/Research/eessd/Terrestrial-Ecosystem-Science and http://tes.science.energy.gov/.

Further information on SBR objectives along with a listing of past and current funding opportunities discussed in this document, is available at https://science.osti.gov/ber/Research/eessd/Subsurface-Biogeochemical-Research.

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Terrestrial Ecosystem SCIENCE

Subsurface Biogeochemical Research

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