

STUDENT ABSTRACTS

Snowmelt-induced hydrologic shifts drive biogeochemical and ecological processes in hyporheic zone environments

Robert Danczak^{1†}, Audrey H. Sawyer², Kenneth H. Williams³, Chad Hobson³, James C. Stegen⁴, Michael J. Wilkins^{1,2*}

¹The Ohio State University Department of Microbiology, ²The Ohio State University Department of Earth Sciences, ³Lawrence Berkeley National Laboratory, ⁴Pacific Northwest National Laboratory

† danczak.6@osu.edu

* wilkins.231@osu.edu (SBR Project Leader)

The hyporheic zone (HZ) is the shallow streambed region of surface water and groundwater mixing that plays a significant role in aquatic nutrient cycling and contaminant removal. Depth-resolved pore water samples were collected through the HZ in the Colorado River near Rifle, CO during periods of high, intermediate, and low river flow. These depth profiles were analyzed for geochemical and microbial changes associated with dynamics in hyporheic mixing. As the river stage receded over the summer, river water did not penetrate as deeply into the subsurface, and HZ chemistry became more anoxic and groundwater-dominated. The microbial community responds to this shifting hydrology, with differing community structures identified during each sampling period. The communities appeared to stabilize through time as groundwater began to dominate the deeper portions of the HZ depth profile with shallower microbial communities beginning to resemble those previously found at depth. Ecological modeling was performed by calculating beta-nearest taxon index (β NTI) and was used to quantify the ecological processes occurring within the HZ during these hydrological disturbances. Modeling revealed a strong deterministic pressure exerted within the HZ across all depths and times, driving communities to be more dissimilar than randomly generated community compositions. Deeper examination of these data revealed that the extent of river water mixing and organic carbon concentration were key factors in selecting for certain community structures over others. These results indicate that the mixing of distinct chemical end-members drives key redox fluctuations across HZs, with associated changes in microbial community composition. Such seasonal effects likely have implications for metal release from sediments, carbon processing, and nutrient cycling in HZ ecosystems.

Authors: Lauren Foster¹, James Beisman¹, Reed Maxwell¹, Lindsay Bearup¹, Ken Williams², Rosemary Carroll³

¹Colorado School of Mines, ²Lawrence Berkeley National Lab, ³Desert Research Institute

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Development of multiple simulation capabilities to model hydrologic partitioning and biogeochemical cycling at the Berkeley Lab's East River Field Site

Berkeley Lab's Subsurface Biogeochemistry Watershed Function SFA seeks to develop a mechanistic understanding of coupled climate-hydrological processes that underlie the ability of mountainous watersheds to retain and release water, nutrients, carbon, and metals. Development of simulation capabilities that describe both flow of water and reactant transformations are sorely needed, as are numerical experiments that predict their response to system disturbance and climate-induced changes. Here, we present two new simulation capabilities utilizing the physically based hydrologic model ParFlow and developed to investigate complexities from the biogeochemical scale up to watershed partitioning: 1) a highly resolved, fully integrated hydrologic model and 2) a new reactive transport model, ParFlow.RT.

The most highly resolved, (2.76M, 10m cells over a 273km² domain), fully parallelized, integrated watershed model from the subsurface through the land surface was built for Berkeley Lab's East River SFA Watershed Study Site. This model provides a platform for numerical experiments studying the influence of climate and vegetation change on hydrologic partitioning and biogeochemical feedbacks. The model was driven to dynamic equilibrium then driven by spatially variable estimates of meteorology at hourly intervals. Model output is compared with field observations to answer questions posed by the Watershed Function SFA. In tandem with field manipulations, these simulations help develop a robust understanding of environmental changes on hydrology. This model is the most highly resolved integrated watershed model in the world to date, allowing for experiments to probe the limits of computational hydrology.

In natural subsurface systems, total elemental fluxes are heavily influenced by areas of disproportionately high reaction rates. These pockets of high reaction rates usually occur at interfaces, such as the hyporheic zone, where a hydrologic flowpath converges with a chemically distinct flowpath or a reactive substrate. Understanding these highly reactive zones is integral to the accurate quantification of nutrient fluxes and biogeochemical cycling in natural systems. Reactive transport simulations can provide information about controls in these highly reactive zones. We have developed a new reactive transport model, ParFlow.RT, by coupling the parallel flow and transport code ParFlow with the geochemical engines of both PFLOTRAN and CrunchFlow. The coupling was accomplished via the Alquimia biogeochemistry library, which provides a unified interface to several geochemical models. Here, we present the details of this new model, and the results of biogeochemical simulations of the Berkeley Lab's East River field site outside of Gothic, CO.

Effect of belowground warming on surface methane and CO₂ fluxes from a boreal black spruce peatland

High latitude peatlands represent a major terrestrial carbon store sensitive to climate change, as well as a globally significant methane source. While elevated atmospheric carbon dioxide concentrations and warming temperatures may increase peat respiration and C losses to the atmosphere, reductions in peatland water tables associated with increased growing season evapotranspiration may alter the nature of trace gas emission and increase peat C losses as CO₂ relative to methane (CH₄). As CH₄ is a greenhouse gas with twenty times the warming potential of CO₂, it is critical to understand how factors associated with global climate change will influence surface CO₂ and CH₄ fluxes. We used an automated soil respiration system at the SPRUCE (Spruce and Peatland Responses Under Climatic and Environmental Change) Experiment to assess the effect of belowground warming on peat CO₂ and CH₄ production throughout the first year of experimental treatment. We use the continuous flux record to assess seasonal and diel flux patterns across the five warming treatments (+0°C, +2.25°C, +4.5°C, +6.75°C, +9°C), and separate the influence of physical (i.e., plant species composition, microtopography) and environmental (i.e., peat temperature, water table position, oxygen availability) factors on observed rates of CH₄ and CO₂ loss. We find that both CO₂ and CH₄ fluxes increased significantly across belowground warming treatments, although CH₄ responded more strongly to temperature increases than CO₂. Peat microtopography strongly influenced trace gas emission rates, and peat hollow locations showed consistently higher CH₄:CO₂ ratios than peat hummocks. Hollow locations also responded more strongly to elevated temperatures throughout the belowground warming component of the experiment. Trace gas production in was also more sensitive to warming than hollow locations than hummocks. While there was no difference in the isotopic composition of the methane fluxes between hollow and hummock locations, $\delta^{13}\text{CH}_4$ was more depleted in the early and late growing season, indicating a transition from hydrogenotrophic to acetoclastic methanogenesis during periods of high photosynthetic input. The measurement record demonstrates that belowground warming has measureable impacts on the nature of peat greenhouse gas loss within one year of treatment onset and highlights the vulnerability of high-latitude wetlands to future temperature increases.

Latitudinal Differences in Peatland Organic Chemistry observed by FTIR, UV/Vis Absorption, and Fluorescence Spectroscopies

Suzanne B. Hodgkins^{a*}, Malak Missilmani^b, Brittany R. Winkler^a, Kelsey Rogers^a, Brittany Verbeke^a, Rachel M. Wilson^a, Jianqing Tian^c, Hongjun Wang^c, Mengchi Ho^c, Neal Flanagan^c, Joumana Toufaily^b, Rasha Hamdan^b, William T. Cooper^d, Jeffrey P. Chanton^a, and Curtis J. Richardson^{c†}

^a Department of Earth, Ocean, and Atmospheric Science, Florida State University, Tallahassee, FL 32306, USA; ^b Laboratory of Materials, Catalysis, Environment and Analytical Methods (MCEMA-CHAMSI), EDST and Faculty of Sciences I, Lebanese University, Campus Rafic Hariri, Beirut, Lebanon; ^c Duke University Wetland Center, Nicholas School of the Environment, Durham, NC 27708, USA; ^d Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL 32306, USA

* Presenting author: sbh10c@fsu.edu. † Principal investigator: curtr12@gmail.com
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The existence of peat deposits at low latitudes, where warm temperatures would be expected to prevent peat accumulation, is thought to be enabled by a combination of phenolic release from plants and the formation of refractory black carbon during low intensity fires. The extent to which these mechanisms may attenuate warming feedbacks in northern peatlands poses a major research question. In this study, we analyzed the chemistry of solid phase peat and dissolved organic matter (DOM) from across a broad latitudinal gradient, which included a thawing permafrost peatland in subarctic Sweden (Stordalen Mire), boreal peatlands in northern Minnesota (Marcell Experimental Forest and Glacial Lake Agassiz Peatlands), a temperate pocosin in North Carolina with frequent fires, a subtropical peatland in the northern Everglades (Loxahatchee), and tropical peat domes in Panama and in Brunei, Borneo. Solid phase peat chemistry was analyzed by Fourier transform infrared (FTIR) spectroscopy, for which novel methods of data analysis are presented. Ratios of peak absorbances to the total spectral area, which reveal quantitative changes in functional group relative abundances, revealed lower carbohydrate and greater aromatic content in southern compared to northern peatlands. Carbohydrates decreased with depth at all sites, and this decrease was accompanied at most sites by increases in aliphatics and slight increases in aromatics with depth. DOM chemistry was examined with UV/visible absorption spectroscopy and excitation-emission matrix spectroscopy (EEMS). Compared to other peatlands, DOM from the Everglades had greater fluorescence/absorbance ratios and absorption spectral slopes consistent with lower molecular weights, as well as shorter fluorescence emission wavelengths consistent with lower aromaticity. This result contrasts with the Everglades' slightly higher solid phase aromaticity compared to northern peat, and suggests that this site's greater minerotrophy may result in greater contribution of recent plant production and microbial activity to the DOM pool. Within the pocosin site, unexpected trends with fire history were observed, in which DOM from locations with recent fires (0–5 years prior to sampling) had lower aromaticity than DOM from a site that had not been burned in 30 years. Overall, the solid phase peat results confirm our hypothesis that southern peat has greater aromaticity and lower carbohydrate content than northern peat. Trends in DOM composition were less straightforward, suggesting that a broader range of factors controls DOM chemistry.

Title: How does deep warming of a peatland affect methane production?

Authors: Anya Hopp¹, Laurel Pfeifer-Meister¹, Jason K. Keller², Cassandra A. Medvedeff², Paul Hanson³, and Scott D. Bridgham¹

Author Organizations: ¹Institute of Ecology and Evolution, University of Oregon, Eugene, OR 97403 USA, ²Schmid College of Science and Technology, Chapman University, Orange, CA 92866, Environmental Sciences Division, Oak Ridge National Lab, Oak Ridge, TN, 97831; ahopple@uoregon.edu

Abstract: Despite covering <3% of the Earth's surface, peatlands contain one-third of total global soil carbon (C) and are responsible for approximately 10% of global methane (CH₄) flux. Methane has a radiative potential 28-times greater than carbon dioxide (CO₂), and the accuracy of Earth system model projections hinges on our mechanistic understanding of peatland CH₄ cycling in the context of environmental change. The objective of this study was to determine, under in situ conditions, how heating of the peat profile affects ecosystem-level anaerobic C cycling. We assessed the response of CO₂ and CH₄ production, as well as the CO₂:CH₄ ratio, in a boreal peatland after four (September 2014) and thirteen (June 2015) months of deep peat heating as part of the Spruce and Peatland Responses Under Climatic and Environmental Change (SPRUCE) project. The study utilizes a regression-based experimental design including five temperature treatments that warmed the entire 2 m peat profile from 0 to +9 °C above ambient temperature beginning in June of 2014. Soil cores were collected at 25, 50, 100, 150 and 200 cm depths from each experimental chamber at the SPRUCE site and anaerobically incubated at in situ temperatures. Rates of CO₂ and CH₄ production were then measured over the course of 1-2 weeks. Methane and CO₂ production in surface peat were positively correlated with seasonal and experimentally elevated temperature ($p < 0.001$), but no consistent temperature response was observed at depth (50-200 cm). Surface peat had greater CH₄ production rates than deeper peat (GLM, $p < 0.001$), implying that the increased CH₄ emissions observed in the field were largely driven by surface peat warming. Additionally, the CO₂:CH₄ ratio was inversely correlated with temperature in the surface and 100 cm depth increments ($p \leq 0.01$), indicating that surficial anaerobic respiration becomes more methanogenic with warming. While SPRUCE will continue for many years, our initial results suggest that the vast C stores at depth in peatlands will be less responsive to warming than surface peat.

Carbon Dynamics of the Greater Everglades Watershed and Implications of Climate Change

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Matthew McClellan¹; Xavier Comas¹; Brian Benscoter²; and Ross Hinkle³

¹: Department of Geosciences, Florida Atlantic University

²: Department of Biological Sciences, Florida Atlantic University

³: Department of Biology, University of Central Florida

Peatlands play a critical role in the carbon (C) cycle in two main ways: 1) by sequestering and storing a large fraction of the global soil C pool; and 2) by producing and releasing significant amounts of greenhouse gasses (CO₂, CH₄) into the atmosphere. While most studies exploring these attributes have traditionally focused on boreal and subarctic biomes, wetlands in temperate and tropical climates (such as the Florida Everglades) have been understudied despite accounting for more than 20% of the global peatland C stock.

To estimate below ground C stocks we use a combination of indirect non-invasive geophysical methods (ground penetrating radar, GPR), aerial imagery, and direct measurements (coring) to estimate the contribution of subtropical depressional wetlands to the total C stock of the pine flatwoods landscape at the Disney Wilderness Preserve (DWP, Poinciana, FL). Three-dimensional GPR surveys are used to define total peat volumes (i.e. from the surface to the mineral soil interface) within five depressional wetlands. Depth-profile cores are used in conjunction with C core analysis to determine changes in soil C content with depth. By combining both GPR and C content variability with depth, a total C stock for each depressional wetland is determined. Aerial photographs are used to estimate surface area for each depressional wetland and develop a relationship between surface area and total wetland C stock. This relationship is then applied to every depressional wetland in the Preserve to estimate total C stock for all depressional wetlands. Additionally, low-frequency GPR surveys prove stratigraphic controls on the development of depressional wetlands by showing collapse structures underneath the depressions that extend to depths exceeding 30 meters.

Spatial and temporal variability in natural greenhouse gas production and release from peat soils in the Preserve has been investigated in several samples at the laboratory scale from three different wetland ecosystems in central Florida (sawgrass peatland, a wet prairie, and a depressional wetland within a pine flatwood). Gas content variability (i.e. build-up and release) within the peat matrix is estimated over a period of five months using a series of high frequency (1.2 GHz) GPR surveys constrained with gas traps fitted with time-lapse cameras. Gas entrapped is analyzed with a gas chromatograph to determine CH₄ and CO₂ content. Additionally, variability in gas build-up and release at high temporal resolution (i.e. sub-hourly) is investigated in a peat monolith using a unique autonomous rail system that provides continuous, uninterrupted GPR transects.

Roots stimulate carbon cycling while mycorrhizae stimulate nitrogen cycling in a boreal upland forest

Jessica A. M. Moore, PhD Candidate

University of Tennessee, Knoxville, TN

Plant roots, their associated mycorrhizal community, and the free-living microbial community interact to regulate the movement of carbon from soil to the atmosphere, one of the most important and least understood fluxes of terrestrial carbon. Our understanding of how plant-microbial interactions alter soil carbon decomposition is lacking, leading to poor model predictions of terrestrial carbon feedbacks to the atmosphere. I tested how roots, mycorrhizal fungi, and the free-living microbial community alter soil carbon decomposition and predicted roots and mycorrhizal fungi would additively increase microbial activity. I manipulated the access of roots and mycorrhizal fungi to bulk soils *in situ* in a boreal upland forest (Marcell Experimental Forest, MN, USA). I added ^{13}C -labelled substrate to trace carbon through respiration and measured microbial extracellular enzyme activity.

I used a structural equation modelling approach to determine how direct and indirect effects of roots and mycorrhizae alter soil microbial decomposition activity and carbon fluxes. The model with the best fit to my field data included a direct effect of roots on carbon-degrading enzyme activity, which was stronger than their indirect effect mediated by microbial biomass. Similarly, I found that the direct effect of mycorrhizal fungi on nitrogen-acquiring enzyme activity was stronger than their indirect effect mediated by microbial biomass. Soil respiration and metabolism of a ^{13}C -labelled substrate was positively correlated with activity of nutrient acquiring enzymes but negatively correlated with carbon-degrading enzymes. Overall, this study demonstrates differences in root and mycorrhizal effects on ecosystem processes. These results provide empirical support for next-generation ecosystem models that describe decomposition rates as a function of roots and mycorrhizal fungi.

Title: Using Optical Oxygen Sensors and Targeted Microbial Analyses to Examine Methane Dynamics in the Boreal Rhizosphere

Authors: Nicholas B. Waldo, Brianna K. Hunt, Heidi L. Gough, Ludmila Chistoserdova, David Beck, Rebecca B. Neumann

Principle Investigator: Rebecca B. Neumann\

Affiliation: University of Washington

Program: SBR

Abstract: Methane is responsible for 15-19% of total greenhouse gas radiative forcing, and natural wetlands are responsible for 20 to 50% of methane emissions. In wetlands, methane is produced in anoxic, saturated soils by anaerobic methanogens from acetate and/or hydrogen produced by fermenters. The anaerobic fermenting microbes must compete with aerobic heterotrophs for organic substrates. These aerobic heterotrophs also compete with aerobic methanotrophs for oxygen. These complicated microbial interactions control the rates of methane production, oxidation, and emission. Spatially, the most interesting region for these processes is the rhizosphere: the region in which soil and groundwater chemistry are significantly impacted by plant roots. Up to 90% of wetland methane is emitted to the atmosphere through plants, and thus, rhizosphere processes can notably influence total methane emissions. As atmospheric carbon dioxide concentrations continue to rise the physiological response of plants, primarily an increase in root carbon exudation, will lead to changes in the rhizosphere and therefore in methane dynamics of the entire wetland system.

This study will examine microbial interactions and methane dynamics in the rhizosphere of *Carex aquatilis*, a wetland sedge, grown under both an ambient and elevated (800 ppm) concentrations of atmospheric carbon dioxide. Ten sedges will be grown under each condition. Oxygen concentrations surrounding the roots of the plants will be monitored throughout the experiment using optical oxygen sensors, and the data from sensors will be used to target fine scale microbial and chemical sampling. Prior to these sampling events we will expose plants to ^{13}C -CO₂ and track the labeled carbon into microbial DNA and various peat carbon pools to quantify the fate of photosynthesized carbon. We hypothesize that plants in the elevated carbon dioxide condition will have increased rates of root carbon exudation, which in turn will stimulate heterotroph activity, causing heterotrophs to outcompete methanotrophs for rhizosphere oxygen and significantly decreasing the percentage of methane oxidized before release to the atmosphere.

Soil carbon inputs and ecosystem respiration: a field priming experiment in Arctic coastal tundra

High latitude soils have been a historical carbon sink due to low decomposition rates in frozen, cold, or anoxic soils. Future soil carbon stocks will depend on the balance between plant carbon inputs and organic matter decomposition, which are both expected to change with warming of high-latitude landscapes. Important to this balance, vegetation and decomposition may interact via the quantity, chemistry, and spatial distribution of plant-derived soil carbon inputs. This study addresses the priming effect, one such interaction whereby increased root exudation alters the background rate of SOM decomposition via microbial biomass increases, co-metabolism of substrates, induced nitrogen limitation, or other possible mechanisms. The priming effect has been observed in numerous laboratory and greenhouse experiments, and there is considerable interest in including this process in ecosystem models. Only few studies, however, have evaluated the priming effect with in situ field experiments. Addressing this gap, we conducted a two-year field experiment in Barrow, Alaska to test for a priming effect under natural environmental variability. In September 2014 and August 2015, we added 1.2g of ^{13}C -labeled glucose to 25cm diameter mesocosms, 15cm below the soil surface in the mineral soil layer. We chose this carbon addition rate to equal an estimated 50% of the layer's microbial biomass carbon. For one month following each substrate pulse, we quantified effects on the rate and temperature sensitivity of background (non-glucose-derived) ecosystem respiration, GPP, and CH_4 emissions. Soil samples were collected twice following each glucose injection, at 1 and 3 weeks in 2014 and 1 and 4 weeks in 2015, for microbial biomass and community composition analysis. Additionally, we buried ion exchange membranes for one week following the 2014 treatment to assess nitrate and ammonium availability. In contrast to many laboratory incubation studies using soils from a broad range of ecosystems, our preliminary results show no significant priming effect. In spite of a clear signal of ^{13}C -glucose decomposition in respired CO_2 , we detected no significant differences in background ecosystem respiration between treatment and control plots. Further analyses will include microbial biomass, microbial community composition, and ^{13}C recovery from soil profiles. This study is part of the Next Generation Ecosystem Experiments (NGEE-Arctic), which aims to improve models of Arctic greenhouse gas fluxes by integrating a broad range of measurements from the cm- to the landscape-scale. To best inform models representing complex and dynamic ecosystems, this study calls for continued research relating theory, laboratory findings, and field experimentation.

Tree species influences phosphatase activity and microbial community composition

Kristine Cabugao^{1,2}, Xiaojuan Yang^{2,3}, Joanne Childs^{2,3}, Collin Timm⁴, Alyssa Carrell⁴, Dave Weston^{2,4}, Richard Norby^{2,3}

¹Bredesen Center, University of Tennessee Knoxville, Knoxville TN 37920, USA

²Climate Change Sciences Institute, Oak Ridge National Laboratory TN 37830, USA

³Environmental Sciences Division, Oak Ridge National Laboratory TN 37830, USA

⁴Biological Sciences Division, Oak Ridge National Laboratory TN 37830, USA

Abstract

Tropical forests are an important carbon sink, responsible for cycling more CO₂ and water than any other terrestrial biome. The goal of the Next Generation Ecosystem Experiments–Tropics project is the synthesis of modeling and data to understand feedback systems that influence terrestrial-atmosphere CO₂ flux. This approach locks modeling and data into an iterative cycle that uses models to identify uncertainties and uses data to improve the model. Reduction of uncertainties in global ecosystem models requires the accurate representation of the tropics, which can be improved by including important belowground processes.

One important belowground process is the biological mineralization of phosphorus, which can be considered a limitation to growth in tropical forests, ultimately influencing CO₂ flux. Parent material determines the initial supply of phosphorus, though the amount of it available for plants is usually much less, requiring the release of phosphatase enzymes to supply the inorganic phosphate (P_i) crucial to their growth.

Three forested sites in Puerto Rico – Rio Icacos, El Verde Ridge, El Verde Valley – were chosen to investigate the effect of parent material on phosphatase activity of four common species: *Cecropia schreberiana*, *Prestoea montana*, *Cyrilla racemiflora*, *Dacryodes excelsa*, and *Manilkara bidentata*. The two El Verde sites, on volcanistic parent material, and the Rio Icacos site on quartz-diorite form a range of conditions helpful to the development of relationships between edaphic factors and phosphatase enzymatic activity. Fine root clusters collected from three trees of each species were assayed for both types of phosphatase activity: phosphomonoesterase and phosphodiesterase. DNA extracted from the rhizosphere and endosphere of fine root clusters within El Verde Ridge and Valley sites were used for 16S rRNA gene profiling of microbial community composition.

Results from two-way ANOVA indicate the importance of species in determining phosphatase activity, particularly of phosphodiesterase. Within the El Verde sites, ANOVA comparisons of phosphatase activity with respect to species also show that species is an important factor. However, only phosphodiesterase activity was significantly different among species within the Rio Icacos site. Microbial community composition, assessed through QIIME, showed a difference between *Dacryodes excelsa* and *Prestoea montana*. Comprehension of how phosphorus constrains ecosystem productivity involves determining how individual trees adjust to their local environment, particularly with belowground processes that enhance phosphorus availability.

EARLY CAREER ABSTRACTS

Nanoscale Mercury Sulfide-Organic Matter Interactions: Practical Applications for Environmental Risk Assessment

Heileen Hsu-Kim, Anh L.-T. Pham, Nelson Rivera

Duke University, Department of Civil & Environmental Engineering, Durham, NC

The geochemical speciation of mercury (Hg) is an important factor that controls the bioavailability of this metal to anaerobic microorganisms responsible for methylmercury production in the aquatic environment. In anaerobic settings, Hg is largely associated with sulfides and natural organic matter (NOM). These interactions involve a variety of species, including Hg complexes with thiolate moieties on NOM and HgS nanoparticles that can be stabilized in solution by NOM coatings. This study aims to delineate how the molecular structure of NOM-coated HgS nanoparticles alters the bioavailability of Hg for methylating microorganisms and to use this information for new methods to quantify Hg bioavailability in sediments and other geomeia.

A variety of spectroscopic techniques was used to delineate the structure of HgS nanoparticles as they aged for up to one week in the presence of NOM. These nanoparticles were then amended to cultures of methylating bacteria. The results demonstrated that the methylation potential of HgS decreased with the age of the nanoparticles, and that this trend coincided with an increase in aggregation and crystallinity of the nanoparticles. The amount of dissolved Hg in solution (defined by the fraction passing a 0.02-micron filter or remaining in suspension after ultracentrifugation) was not a good predictor of Hg bioavailability. Instead, bioavailability correlated with the fraction of particulate Hg that dissolved in the presence of glutathione, a thiolate ligand that could be representative of metal binding sites on the bacterial cell envelope. These observations have been used to develop a thiolate-based selective extraction assay for quantifying metal bioavailability in geomeia. Overall, the results of this work suggest that a portion of solid-bound mercury is bioavailable to microorganisms, the reactive fraction depends on the nanoscale structure of HgS, and this fraction can be approximated by a selective extraction assay that can sufficiently mimic processes at microbe-mineral interfaces.

Methane Flux and Oxidation in a Thermokarst Bog in Interior Alaska: The Role of Plants

Rebecca B Neumann¹, Colby J Moorberg², Andrea Wong¹,
Mark P Waldrop³, Merritt R. Turetsky⁴

1. University of Washington
2. Kansas State University
3. United States Geological Survey
4. University of Guelph

Methane is a potent greenhouse gas, and wetlands represent the largest natural source of methane to the atmosphere. A majority of the emitted methane travels through hollow aerenchyma tissues inside emergent plants, which also support the diffusion of atmospheric oxygen down to the rhizosphere. Previous studies have shown that oxidation of methane by oxygen released into the rhizosphere by plants is capable of converting ~90% of CH₄ produced within wetlands to CO₂. Most current large-scale wetland models represent rhizospheric methane oxidation as a constant percentage (i.e., 40–50%) of the methane transported by plants. Oxidation is an important methane sink and changes in the rate of methane oxidation can affect wetland methane emissions. In a thermokarst bog located in Interior Alaska, we conducted a series of measurements and experiments to clarify the impact that plants in this system have on rates of methane oxidation. On individual *Carex* plants isolated in a plant-flux chamber, we measured rates of both plant-mediated methane emission and methane oxidation; we assessed methane oxidation by measuring methane flux after removing oxygen from the flux chamber. After accounting for *Carex* density at the plot scale, we estimated that ~40% of emitted methane traveled through plants. However, we detected minimal to no methane oxidation along the plant-transport pathway. In conjunction with the plant-level flux measurements, we conducted a plant manipulation experiment where we tracked rates of methane emission and methane oxidation on treatments with natural vegetation, with vascular plants removed, and with vascular plants removed and “replaced” with gas permeable tubing. We found that the treatment with the natural vegetation had increased rates of methane emission and, surprisingly, decreased rates of methane oxidation relative to the two other treatments. We hypothesize that plant carbon inputs not only fuel methane production but also provide substrate for heterotrophic microbial communities that compete with methanotrophs for oxygen, thus diminishing the availability of oxygen for methane oxidation. This hypothesis is supported by data collected from *in situ* oxygen injection experiments conducted against optical oxygen sensors installed in the bog against both naturally vegetated peat and peat with vascular plants removed. Over the season, in the shallow depths (~15 cm) oxygen consumption rates were generally faster in the presence of plants. Collectively, these data indicate that in the studied thermokarst bog, not only is minimal to no methane oxidation occurring in the rhizosphere of plants, but plants are decreasing rates of methane oxidation.

Towards a Mechanistic Understanding of Land-Atmosphere Interactions of Reactive Oxides of Nitrogen (DE-SC0014443)

Jonathan D. Raff

School of Public and Environmental Affairs and Department of Chemistry, Indiana University
Bloomington, IN 47405-2204

Global soils are known to be a major source of oxides of nitrogen to the atmosphere. While these emissions have traditionally been associated with nitric oxide (NO) and nitrous oxide (N₂O), recent laboratory measurements and satellite-global model comparisons suggest that nitrous acid (HONO) and nitrogen dioxide (NO₂) may also be an important constituent of the N-budget. Unfortunately, the processes controlling these emissions are not understood due to challenges in elucidating details of the relevant abiotic and biogenic processes occurring within the terrestrial environment. This is especially true for soil microbial emissions of reactive nitrogen (e.g., NO, NO₂, and HONO)—gases that directly and indirectly affect climate by controlling the oxidative capacity of the atmosphere, lifetime of greenhouse gases, and formation rate of aerosols. In this presentation, I will discuss recent progress made in understanding the abiotic and biogenic processes that determine the fate of HONO in soil. We carried out kinetics studies using a coated wall flow reactor and surface composition studies using nano-DESI and nanoSIMS [at the Environmental Molecular Sciences Laboratory (EMSL)] to investigate the role that minerals and organic matter play in storing and releasing HONO in soil. In addition, mesocosm experiments were conducted to characterize the biogenic mechanisms of reactive nitrogen release from agricultural and urban soil. Flux chamber experiments on agricultural and urban soil samples were carried out to identify soil that emitted reactive nitrogen. The biological nature of these emissions was probed in a series of amendment (NH₄⁺ and/or nitrapyrin) studies; 16S rRNA genes and expressed rRNA from the samples were sequenced to provide information on the microbial community composition and activity. Finally, I will describe a newly developed soil flux chamber array that will be used to measure reactive nitrogen fluxes in a northern hardwood forest during a one-month field campaign at the University of Michigan Biological Station in July 2016. This will provide us with the opportunity to field test hypotheses formulated in the laboratory; the results will be used in parameterizations of soil reactive nitrogen flux in future chemical transport models.

The DOE Joint Genome Institute: A dedicated user facility for environmental & energy genomics

Adam R. Rivers

The Joint Genome Institute is a DOE user facility that provides researchers from around the world access to advanced sequencing and analysis, enabling them to address important questions in the areas of bioenergy, carbon cycling and biogeochemical cycling. Each year we solicit large- and small-scale community science program (CSP) proposals. Large-scale proposals are typically complex studies that integrate multiple data types including genome sequencing, metagenomics, metatranscriptomics and single cell analysis. Twice a year we review small scale CSPs and allocate sequencing based on brief white paper proposals. JGI also works with the DOE's Environmental Molecular Science Laboratory to fund projects that combine the unique capabilities of these labs to solve more focused, high-risk/high payoff problems in bioenergy. We continue to develop new analytical capabilities in sequence analysis and in emerging areas including DNA synthesis and metabolomics. JGI also conducts research in terrestrial carbon cycling, plant genomics and plant-microbe interactions. This combination of user and internal science are an important resource for environmental system science.

River bank erosion, lateral accretion of material, and overbank deposition contribute to the exchange of organic carbon (SOC) between alluvial rivers and floodplains. These exchanges, however, are not currently accounted for in the carbon budget of inland waters. We used satellite imagery and historical aerial photographs to quantify rates of bank erosion and floodplain accretion for eleven arctic rivers with drainage areas ranging from 12,000 km² to 2.5 million km². We extrapolated these measurements to compute the river/floodplain exchange of sediments across permafrost-dominated alluvial rivers in the Arctic and subarctic. We then used the Northern Circumpolar Soil Carbon Database to estimate the quantity of SOC carbon entering these rivers from the upper 3 meters of permafrost-dominated floodplain soils. Preliminary estimates indicated that bank erosion in the downstream-most 1,000 km of the Lena River contribute 2 Tg C and 68 Tg sediment per year to the river. These quantities are 2 and 3 times the fluxes C and sediment measured at the delta suggesting significantly more carbon is cycled along arctic river systems than is exported to their deltas.

Computational Bayesian Framework for Quantification of Predictive Uncertainty in Environmental Modeling

DOE Early Career Award DE-SC0008272
Subsurface Biogeochemical Research Program

PI: Ming Ye (mye@fsu.edu)

Department of Scientific Computing, Florida State University, Tallahassee, FL 32306

A computational Bayesian framework has been developed for quantification and reduction of uncertainty in environmental modeling. In this year of the project, the framework is used for both theoretical studies and practical applications.

The theoretical studies are focused on defining new metrics for two sensitivity analyses. The first one is to avoid biased selection of important parameters, which are important only to a single model but not the system of interest if the single model does not represent the system. This is done by defining new sensitivity indices after expanding the variance-based sensitivity analysis of a single model and a single scenario to the framework of multiple models and multiple scenarios developed in this project. To reduce the computational cost for calculating the new sensitivity indices, the sparse grid stochastic collocation method is used to evaluate the statistical moments needed for the indices. The use of the new sensitivity index is demonstrated in a numerical example of groundwater flow reactive transport modeling, which also demonstrates the dramatic reduction of computational cost. The other sensitivity analysis uses the same framework but to select important processes of an environmental model. New process sensitivity indices are defined for the situation that a process can be represented by more than one model. The new indices answer the question that how to select the important processes when it is uncertain how to model the processes. This new method of sensitivity analysis should be of particular use at the early stage of model development when the process model uncertainty is the largest.

Computational advance has been made for evaluating Bayesian evidence using the sparse grid methods. The Bayesian evidence is critical for evaluating relative plausibility of multiple models; a more plausible model has larger Bayesian evidence. Evaluating it however is computationally challenging, because it requires calculating a multivariate integration. This is done in this project using the thermodynamic integration and stepping stone methods. To reduce the computational cost, the sparse grid methods are used to build cheap-to-evaluate surrogates of computationally demanding models. The Bayesian evidence is evaluated for several reactive transport models for identifying the right level of model complexity.

By collaborating with scientists at the Pacific Northwest National Laboratory, we have applied our new methods of sensitivity analysis for the Hanford 300 Area to select important parameters. Collaboration with scientists at the Oak Ridge National Laboratory is on-going for identifying important processes of climate change modeling. The collaboration of mutual interests help improve the methodology development and gain insights for practical problems.

AMERIFLUX ABSTRACTS

AmeriFlux Carbon Flux Data System

Margaret Torn¹, Gilberto Pastorello¹, Deb Agarwal¹, Boris Faybishenko¹, Marty Humphrey², Norm Beekwilder², Thomas Boden³, Housen Chu⁵, Bai Yang³, Megha Sandesh¹, You-Wei Cheah¹ and Dario Papale⁴

¹Lawrence Berkeley National Laboratory, ²University of Virginia, ³Oak Ridge National Laboratory, ⁴Tuscia University, ⁵University of California, Berkeley

The AmeriFlux network brings together independently managed field sites, measuring concentrations and fluxes of carbon, water, and energy across the Americas. The data are processed into fluxes, quality controlled, and sent to the AmeriFlux network for publication. The data management team is working to harmonize data and metadata formats, perform QA/QC, and build data processing pipelines in collaboration with the European ICOS and other regional networks. The main goal of the effort is to enhance data synthesis, land model evaluation, and other multi site data applications.

The data team has recently standardized the data and metadata formats that are incorporated in new releases of standardized sets of flux-data products (featuring gap-filling, GPP/respiration partitioning, and uncertainty assessments products). Changes to variables reflect new developments in flux data collection and were designed to better support data/metadata sharing. These changes are also a milestone in terms of international harmonization and represent a crucial step to facilitate global use of eddy covariance data that are acquired under different regional networks. We are generating derived and value-added data products from data but putting data through a series of quality checks and post-processing steps. A concentration in the last year and for the future will be development and improvement of this processing pipeline. New releases of standardized sets of flux data products (featuring gap-filling, GPP/respiration partitioning, and uncertainty assessments products) have been produced for the first time since the LaThuile dataset in 2007., and released as FLUXNET2015. We have also made significant changes to the BADM (Biological, Ancillary, and Disturbance Metadata) protocols, to facilitate data reporting and site search.

Title: AmeriFlux Management Project Tech Team

Sébastien C. Biraud¹, Stephen W. Chan¹, Sigrid Dengel¹, Chad Hanson², Dave Billesbach³, Margaret S. Torn¹

¹Lawrence Berkeley National Laboratory, ²Oregon State University, ³University Nebraska Lincoln

Abstract:

AmeriFlux's goal is to develop a network of long-term CO₂ flux sites for quantifying and understanding the role of the terrestrial biosphere in global climate change. The network currently includes more than 100 sites started by many scientists and supported by multiple agencies (DOE, NSF, USDA, NFS). The AmeriFlux Management Program (AMP) Technical QA/QC at LBNL strengthens the entire AmeriFlux Network and Core Sites by—

- standardizing operational practices, calibration, and maintenance routines,
- setting clear data quality goals,
- helping resolve instrument failure promptly.

To ensure inter-comparability in the network, we conduct site comparisons with portable eddy covariance (PEC) systems, provide calibration gas standards and lab-quality sensors to check instrument performance, and identify uncertainties associated with data processing using data diagnostics and gold-standard files.

Our team is experienced in testing new instruments and working with manufacturers, and is building relationships with both vendors and investigators. We have completed 17 QA/QC site visits in since the beginning of the project

TITLE:

The AmeriFlux Management Project

AUTHORS:

Margaret Torn, Deb Agarwal, Sebastien Biraud, Trevor Keenan, Marilyn Saarni, and Dennis Baldocchi

ABSTRACT TEXT

In 2016, AmeriFlux will celebrate its 20th year as a close-knit network of independent eddy covariance sites across the Americas, measuring terrestrial ecosystem carbon, water and energy fluxes. The primary goal of LBL's AmeriFlux Management Project (AMP) is to optimize quality of AmeriFlux data and its use by a broad community. We are working to expand the network's role as a virtual field laboratory for basic research and Earth System Model (ESM) improvement, and to facilitate innovative measurements and data synthesis. To achieve these goals cost-effectively, we set up teams to cover four tasks: (1) Core site support; (2) Technical support and QA/QC; (3) Data support and QA/QC in coordination with the Carbon Dioxide Information and Analysis Center (CDIAC); and (4) Outreach. In AMP's first three years, we funded operations for 14 clusters of long-term flux sites, established comprehensive tech support, enhanced data services, revived annual AmeriFlux meetings and Science Steering Committee, and built collaborative relationships with the AmeriFlux community, and ICOS (Europe) and FLUXNET (global) networks. We will continue these activities, and deliver: (1) consistent operations of high quality, longterm Core sites; (2) expanded data holdings for sites in boreal, arctic, and other poorly represented ecosystems; (3) enhanced data QA/QC and technical support to the AmeriFlux network; (4) the first new gap-filled, partitioned synthesis dataset since 2007, which will enable next-generation models, synthesis, and research activities; (5) outreach that strengthens the AmeriFlux community, raises its visibility, and boosts the next generation of Earth scientists. This poster will illustrate the main AMP activities and highlights recent exciting results from the AmeriFlux network."

EMSL ABSTRACTS

EMSL: A DOE Scientific User Facility for Terrestrial and Subsurface Science Research

Nancy Hess, Science Lead for Terrestrial and Subsurface Ecosystems

Environmental Molecular Sciences Laboratory (EMSL) See: <http://www.emsl.pnl.gov/>

Robust, predictive models of elemental cycling and contaminant fate and transport in the subsurface require understanding and identification of key geochemical and biogeochemical reactions that control species reactivity and mobility at multiple scales. The ability to identify and adequately probe dynamic processes at the molecular to pore scale can provide information needed to accurately simulate these processes with computational models and incorporate them into reactive flow and transport models, an important goal of many Environmental System Sciences researchers who address the nation's environmental and energy challenges. Linking of experimental and theoretical information from molecular to field scale requires the convergence of diverse experimental and computational techniques and collaboration with experts from multiple disciplines.

EMSL, a DOE national user facility in Richland WA, provides integrated experimental and computational resources and expertise for scientific studies and discovery in subsurface biogeochemical research to users free of charge. There are numerous capability sets that are particularly relevant for biogeochemical research. I) Next generation imaging and surface characterization experimental capabilities can be used to provide the spatially resolved elemental analysis, oxidation state determination, chemical speciation, mineral identification, and microbe-mineral associations necessary for understanding the chemical fate and mobility of contaminants in the biogeochemical environment. II) Advanced spectroscopic capabilities are used for determining the speciation of metal ions and complexes on surfaces, in solution, or incorporated into mineral phases. III) Comprehensive quantitative proteomics/metabolomics platforms, whole transcriptome analysis platforms, platforms for gene expression profiling, small RNA analysis, novel transcript identification, and many genome- and epigenome-directed applications provide EMSL users extensive capabilities for unraveling the interplay between microbial communities and geochemistry. IV) An integrated suite of capabilities to support research in subsurface flow and transport provide data from the micron to the intermediate scale. Users have access to experts who assist with all steps of the research process from pre-experiment modeling to hydraulic characterization, numerical modeling, and post-process analysis on custom-built flowcells.

RadEMSL, EMSL's radiochemistry annex, greatly expands the range of experimental capabilities for analysis of environmental samples contaminated with radionuclides, is now available to users. The new facility consists of approximately 6000 sq ft of lab space. The surface analysis-imaging suite contains FIB-SEM, TEM-EELS, SPM, XPS, and EMP. The Magnetic Resonance Facility houses 100 and 750 MHz wide-bore NMR spectrometers, with a wide range of specialized sample environments and nuclide probes, as well as an EPR spectrometer. The Radiochemistry Annex also houses sample preparation, solution chemistry and analytical tools including XRD and fluorescence capabilities. These capability sets together with NWChem, EMSL's premier computational modeling code, and a suite of other numerical models of fluid flow and biogeochemical reactions (at molecular, pore, core and ecosystem scales), enable users to address subsurface biogeochemical research challenges from both experimental and modeling vantage points.

Exploring the Soil Microbiome and Elemental Cycling via Advanced Mass Spectrometry at EMSL

Ljiljana Pasa-Tolic, Malak M. Tfaily, Galya Orr, Jared Shaw, Lawrence Walker, Nikola Tolic, Yina Liu, Albert Rivas Ubach, Rosalie Chu, Christopher Anderton, Errol Robinson, Nancy J. Hess

Given that over 90% of microbial community members cannot be cultivated (and thus have unknown functions and identities), together with exceptional diversity and lack of representative assembled genomic databases, microbiome omics data is extremely challenging to acquire, analyze and interpret, particularly with temporal and spatial resolution needed to decipher functional roles within the microbiome. Additionally, a limited understanding of the molecular composition and dynamics of natural organic matter (e.g. soil or dissolved organic matter) within microbial habitats limits our ability to interpret (bio)(geo)chemical processes within complex matrixes (e.g. soil). Therefore, successful development of molecular profiles that link soil microbiology with soil carbon (C) to ascertain soil vulnerability and resilience to climate change would have great impact on assessments of the soil ecosystems and their response to climate change. Fourier transform ion cyclotron resonance (FTICR) offers the highest mass resolving power and accuracy of any mass analyzer; nevertheless, even higher resolution and accuracy is required to capture the full range of information for increasingly complex natural mixtures (e.g., soil organic matter) and biological complexity (e.g., proteomics, metabolomics, metallomics). Herein, we will describe advanced mass spectrometry (MS) capabilities available at EMSL, a DOE national scientific user facility located at PNNL, to address the key knowledge gaps in functional understanding of how complex microbiomes influence and are influenced by their environment and present selected applications to oceanic, freshwater and soil microbiome field studies. Special emphasis will be on the novel high magnetic field (i.e. 21T) Fourier transform ion cyclotron resonance (FTICR) mass spectrometer recently brought online at EMSL. This capability will arguably provide that next level of performance needed to understand e.g. chemistry and dynamics of the belowground carbon cycle. Identification and quantitation of intact molecular structures derived from higher plants and soil microbiome within their native 3D inorganic soil matrix are essential for advancing molecular-scale mechanistic understanding of the role of physical, geochemical, and biological processes belowground. 21T FTICR platform will dramatically increase spectral acquisition rate and attainable sensitivity, and thus enable characterization of intact molecular structures in soil (and other complex matrixes) while addressing spatial relationships and heterogeneity, particularly in combination with other imaging modalities, e.g. FISH and/or nanoSIMS.

SBIR ABSTRACTS

Subsurface system behavior is driven and controlled by the interplay of physical, chemical, and biological processes which occur at multiple temporal and spatial scales. Timely predictive understanding of this behavior is needed for scientific purposes and for system management – whether this is for subsurface remediation, ecosystem services optimization, or water and soil management. Current approaches to develop system understanding generally rely on manual approaches for data reduction, numerical modeling and data visualization. Such approaches have fundamental limitations in how timely, effectively and reproducibly they can provide the required understanding. In addition, manual approaches are ill suited for dealing with the large volumes of heterogeneous (and often streaming) data which are increasingly available for subsurface systems.

Under a DOE SBR funded Phase II SBIR Subsurface Insights has implemented a cloud based predictive assimilation framework (PAF) which can ingest and store heterogeneous subsurface data and can visualize and process this data to provide information on the current state and evolution of the subsurface system. PAF has its roots in web based data management applications developed in support of DOE IFRC projects, but has been refactored and enhanced substantially in response to user needs in the private sector.

PAF is implemented as a modular Zend Framework 2 Web application which is organized around five integrated functions: (1) data acquisition, (2) data management, (3) data assimilation and processing, (4) visualization and result delivery and (5) orchestration. PAF is accessed using a browser, with rich client side interactive capabilities being provided through CSS/Javascript. Back end functionality is provided by python workflows.

PAF organizes its data by projects (where a project typically corresponds to a field site). All sites share the same back end database architecture, where use of the different elements of this architecture depends on the data available within a project. PAF is thus project agnostic, which allows for easy scaling and project deployment. Users can be members of different projects, and have privileges which can be assigned by a project administrator.

Responsiveness of PAF (a major concern in web applications) is achieved by implementing high level PAF capabilities as SPA (Single Page Application). This approach allows for relative simple system development and maintenance.

PAF has been developed in collaboration with LBNL SFA2 scientists and has been tested and demonstrated using hydrological, geochemical and geophysical data data from the Rifle and East River sites. PAF is seeing increasing acceptance in the private sector.

DOE LAB ABSTRACTS

Pore- to Core-Scale Research to Inform Ecosystem-Scale Soil C Biogeochemistry

VL Bailey, B Bond-Lamberty, C Liu

The spatial separation of soil organic carbon (SOC), microbes, and extracellular activity is an important mechanism of SOC protection in soils and is difficult to represent in predictive models at ecosystem scales. **Our overarching science objective is to develop the mechanistic understanding of how SOC in protected locations is metabolized as a result of pore-scale changes in its bioavailability, and to test that understanding using ecosystem models.** We address this objective by integrating modeling, observations, and experiments, using new tools to strengthen team collaboration, and increase transparency and reproducibility, and making our data openly available. Our research, based on experiments using intact and manipulated soil cores from hydrologically dynamic research sites in central Florida and interior Alaska, indicates that the physical protection of SOC breaks down when pedogenic soil structure deteriorates or pores connect hydrologically. Pore- and continuum-scale flow and reactive transport models have been developed to simulate the physical protection of SOC, to evaluate how pore-scale water saturation and hydrological connection in heterogeneous soils affect microbial respiration of SOC, and to establish macroscopic effective relationship between SOC respiration rate and moisture content in soils. Because the soil structural controls on these pore-scale mechanisms strongly correlate to soil texture, we are also evaluating the power of soil texture indicators in global databases for predicting carbon turnover and respiration at much larger scales. By linking experimental data and mechanism-based models with an analysis of ecosystem-scale models, we hope to inform new mechanistic models of C transformation and transport in soils, improve the predictive power of larger-scale models, and address important Terrestrial Ecosystem Science Program goals.

ABSTRACT

Effects of atmospheric warming and precipitation reduction on the interaction between carbon and nitrogen in forest ecosystems

Climate change is expected to increase atmospheric temperatures and modify precipitation regimes with negative consequences on the performance and survival of forest ecosystems. The carbon and water mechanisms of mortality have been extensively studied; however, under current debate is the role of nutritional status on the performance of trees under climate change. It is highly likely that a negative impact of drought and heat on tree nutritional status could play a significant role in the performance of forests. Yet, bridging the gap between nitrogen and the more well studied carbon and water components of drought-induced mortality has not been attempted.

This project is aimed at quantifying the influence of climate change on the link between nutrient, water and carbon relations in forests. For this purpose, we will measure the key processes of the nutrient cycle in trees exposed to reduced precipitation, atmospheric warming and their simultaneous effects. Underlying processes affecting tree nutrient uptake and use will be measured to obtain a mechanistic understanding of the impact of climate change on tree nutritional status. Measurement of key processes of the water and carbon cycle will be simultaneously measured to determine the link between nutrient and carbon relation, in other words, to quantify the consequences of climate-induced changes in nutrient uptake and use.

Knowledge acquired during this experiment will enable the completion of current conceptual frameworks, as well as provide information for climate-vegetation modelers who rarely consider the link between nutrient and carbon relations in forest decline under climate change.

Terrestrial Carbon Cycling: Insights Gained through Radiocarbon Analysis and Interpretation at SPRUCE, Ngee-Arctic, and AmeriFlux

Karis J. McFarlane
Center for Accelerator Mass Spectrometry
Lawrence Livermore National Laboratory

Understanding and modeling terrestrial carbon cycles is a key goal for BER. Radiocarbon is a valuable tool for determining the transit time of carbon in the terrestrial biosphere and for tracking carbon as it moves into, through, and out of ecosystems. In many systems, particularly those in high latitudes, radiocarbon can be used to identify the mobilization and loss of carbon from the large, old reservoirs found in soils including peat and permafrost. This poster highlights recent work applying radiocarbon and other Lawrence Livermore National Laboratory capabilities to BER-related research efforts in terrestrial carbon cycling. Current work at SPRUCE focused on carbon accumulation and the source of emitted methane and carbon dioxide with short-term experimental warming and highlights from recent work on dissolved organic carbon age and chemistry at the Ngee-Arctic Phase I site in Barrow, Alaska will be presented. New efforts to constrain soil carbon turnover and cycling at AmeriFlux sites through data synthesis, reanalysis, and model-data comparison will also be included.

Toward a better prediction of water stress on vegetation dynamics in Earth System Models

Chonggang Xu¹, Sanna Sevanto¹, Turin Dickman¹, Henry Adams¹, Adam Collins¹, Wei Liang¹, Rosie Fisher², Nate McDowell¹

1: Earth and Environmental Sciences Division, Los Alamos National Laboratory, NM;

2: Climate and Global Dynamics, National Center for Atmospheric Research, Boulder, CO.

Forests play a key role in regulation of the global carbon cycle and climate; however, they could be subjected to substantial drought risks in the future due to global warming. Currently, all Earth system models (ESMs) use very few plant functional types (PFTs) with fixed plant characteristics and very limited representation of plant physiology in response to drought. This over-simplification prevents mechanistic and accurate simulation, particularly in the hyper-diverse tropical forests, and may result in over- or under-estimates of forest responses to droughts. In this study, we compared different process-based tree mortality models based on carbon starvation, plant hydraulic failure and phloem failure for the prediction of tree mortality at a drought experiment site in New Mexico under current and future climate conditions. Our results showed that, compared to the simple growth efficiency model, the process-based model better represents the timing of mortality; however, additional data are still needed for accurate predictions of traits that control the key mortality processes under novel climate conditions. There is a strong need for a trait coordination and trade-off model to better predict future vegetation dynamics under droughts across regional and global scales.

NGEE ARCTIC ABSTRACTS

Wetter or drier? A model intercomparison of soil moisture and runoff predictions in permafrost landscapes

Christian G. Andresen¹, Cathy J. Wilson¹, David Lawrence², David A. McGuire³

¹*Los Alamos National Laboratory, Los Alamos, NM;*

²*National Center for Atmospheric Research, Boulder, CO;*

³*U.S. Geological Survey, Alaska Cooperative Fish and Wildlife Research Unit, University of Alaska Fairbanks, Fairbanks, AK.;*

With the predicted loss of permafrost, there is a large uncertainty in future predictions of hydrological conditions across the Arctic. Since hydrology plays a fundamental role in biogeochemical cycles and potential climatic feedbacks, there is a need to better understand how models represent permafrost hydrology and how different representations affect wetting and drying of permafrost landscapes. This study aims to advance understanding of where, when and why the arctic will become wetter or dryer in the soil column. In particular, we assessed and compared models predictions of the spatial and temporal distribution of soil moisture and runoff across permafrost regions and geographical domains (e.g. Boreal N. America, Boreal Europe, etc.) and highlighted the main factors responsible for observed changes. Then, we evaluated fundamental differences in how models simulate soil moisture and runoff. This study serves as a baseline to improve conceptual issues of arctic and boreal hydrology among models and reduce uncertainty in predictions. In addition, this study highlights the need for developing and improving benchmark datasets with seasonal dynamics to evaluate model responses in the permafrost region.

Conceptualization of Intermediate- to Large-scale Parameter Estimation of Landscape Transitions Using Proper Orthogonal Decomposition Techniques

W. Robert Bolton¹, Vladimir Romanovsky², and Mark Lara³

¹ *International Arctic Research Center, University of Alaska Fairbanks, Fairbanks, Alaska, USA*

² *Geophysical Institute, University of Alaska Fairbanks, Fairbanks, Alaska, USA*

³ *Institute of Arctic Biology, University of Alaska Fairbanks, Fairbanks, Alaska, USA*

E-mail address of corresponding author: bbolton@iarc.uaf.edu

Thermokarst topography forms whenever ice-rich permafrost thaws and the ground subsides due to the volume loss when excess ground ice transitions to water. Changes in the landscape due to thermokarst subsidence, even on the order of a few centimeters, can result in profound changes to the drainage dynamics with subsequent shifts to both energy and carbon fluxes. The Alaska Thermokarst Model (ATM) is a meso-scale, state-and-transition model designed to simulate landscape transitions between [non-]thermokarst landscape units, or cohorts. The ATM uses a frame-based methodology to track transitions and proportion of cohorts within a 1-km² grid cell. The transition from one cohort to another due to thermokarst processes can take place if thaw reaches ice-rich ground layers either due to pulse disturbance events such as a large precipitation event or fires or due to gradual active layer deepening that eventually results in penetration of the protective layer. The protective layer buffers the ice-rich soils from the land surface and is critical to determine how susceptible an area is to thermokarst degradation. The frame-based methodology of tracking transitions between landscape units is conceptually consistent with the watershed delineation approach being developed the ALM (ACME Land Model). In the NGEE-Arctic Phase 2 study, we will utilize and apply the recent NGEE-Arctic POD-MM (Pau et. al. 2014; 2015) and POD-GPR (Lui et. al. 2015) approaches to translate the intermediate-resolution modeling results into functional responses applicable for integration into CLM. In the presentation, we present a conceptualization of this upscaling approach that will be implemented in NGEE-Arctic Phase 2.

The Alaska Arctic Vegetation Archive: A report on the status of the Arctic Vegetation Archive and an application in northern Alaska

Abstract:

An overarching goal of NGEE Arctic is to improve our pan-Alaskan, and ultimately pan-Arctic, understanding and modeling of tundra ecosystem processes. To this end, we contributed vegetation data collected from Barrow, Alaska in Phase 1 of NGEE Arctic to the Arctic Vegetation Archive (AVA). AVA is a vegetation-plot database for the Arctic tundra biome with goals of uniting and harmonizing circumpolar Arctic vegetation data and applying the data to an Arctic vegetation classification, ecosystem and biodiversity models, management of Arctic resources, and Arctic education. High quality plot data and non-digital legacy datasets that are in danger of being lost have the highest priority for inclusion in the archive. A PanArctic Species List (PASL) provides a standard list of accepted vascular plant, bryophyte, and lichen species names. Work on the AVA is being accomplished within individual Arctic countries. Here we report progress on an Alaska prototype for the AVA and provide a preliminary analysis of the data currently in the Alaska-AVA.

The Alaska-AVA is accessible to scientists and the public via the Arctic Alaska Geocological Atlas, an on-line resource being developed by the Alaska Geobotany Center and the Geographic Information Network of Alaska at the University of Alaska Fairbanks. The Alaska-AVA utilizes the Turboveg for Windows database program and follows protocols developed for the European Vegetation Archive. Species cover data and ancillary data, including environmental, soils and spectral data, photos, maps, and publications are linked to each plot's geographic location. Approximately 5,000 vegetation plots in northern Alaska are being evaluated for inclusion in the Alaska AVA. These data will also be archived in the ORNL-Distributed Archive Active Center, VegBank, the Ecological Society of America's Panel on Vegetation Classification's vegetation plot database, and referenced through the Global Index of Vegetation Databases (GIVD). Approximately 2,000 plots from 20 separate studies have been imported thus far, including NGEE Arctic vegetation plot data from Phase 1.

A preliminary vegetation analysis is presented that focuses on regional-level vegetation changes along a gradient traversing the three Arctic bioclimate subzones, and three major physiographic provinces, in northern Alaska. Changes along key environmental gradients (summer temperature, soil moisture, soil pH, snow) are examined using multivariate methods. Vegetation classification and variability of habitats across the study area will be discussed. Relationships among plant community composition and environmental gradients across Alaska, and ultimately the Arctic, will provide important model benchmarks for the next generation of models developing under NGEE Arctic.

Biogeochemical Controls on Microbial CO₂ and CH₄ Production Across Polygonal Arctic Soils and Permafrost

David E. Graham^{1,3}, Jianqiu Zheng¹, Taniya Roy Chowdhury^{1,4}, Ji-Won Moon¹, Ziming Yang², Liyuan Liang², Baohua Gu², and Stan D. Wullschleger^{2,3}

¹ Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN

² Environmental Sciences Division, Oak Ridge National Laboratory

³ Climate Change Science Institute, Oak Ridge National Laboratory

⁴ Present Address: Pacific Northwest National Laboratory, Richland, WA

Contact: D. Graham (grahamde@ornl.gov)

Abstract

Warmer Arctic temperatures are increasing the annual soil thaw depth and prolonging the thaw season in Alaskan permafrost zones. This change exposes organic matter buried in the soils and permafrost to microbial degradation and mineralization to form CO₂ and CH₄. The proportion and fluxes of these greenhouse gases released into the atmosphere control the global feedback on warming. To improve representations of these biogeochemical processes in terrestrial ecosystem models for the Next-Generation Ecosystem Experiments in the Arctic (NGEE-Arctic) project, we compared physico-chemical properties and microbial activities in soil core samples from three classes of ice-wedge polygons from the Barrow Environmental Observatory in Barrow, AK. High-centered, flat-centered and low-centered polygons represent a gradient of permafrost-affected tundra with increasing water saturation. The soil water potential in high- and low-centered polygon soil layers was determined. Matric potential along with temperature likely explains porewater freezing, gas diffusion and microbial activity.

The temperature-dependent CO₂ and CH₄ production from anoxic soil incubations at -2, +4 or +8 °C identified a significant lag in methanogenesis relative to CO₂ production by anaerobic respiration and fermentation. Proportions of the two greenhouse gases varied substantially across microtopographic positions and soil horizons. The abundance of methanogen signature genes increased during incubations. CH₄ oxidation was observed in microcosms containing soils from all horizons from both high-centered and flat-centered polygons, and prolonged thawing significantly accelerated CH₄ oxidation rates. Comparisons of samples collected across the microtopographic polygonal features address the impacts of water saturation, iron reduction and organic matter content on CH₄ production and oxidation. These combined measurements build process understanding that can be applied across scales to constrain key response factors in models that address Arctic soil warming.

Fine-scale modeling of permafrost using the Advanced Terrestrial Simulator

Data collected by the NGEE Arctic team at the Barrow Environmental Observatory (BEO) is refining the Advanced Terrestrial Simulator (ATS) and, conversely, ATS is informing field studies. Through this ModEx strategy, the fine scale modeling team and collaborators in NGEE Arctic are gaining understanding of permafrost change in a changing climate. The ATS is a hydrothermal model built using a modern modular computational framework to address complex multi-physics problems, which includes a snow surface energy balance, coupled with a variably saturated subsurface thermal hydrology model.

Our modeling has improved our understanding of fine-scale processes in the Arctic permafrost and identified fine-scale phenomena that have large-scale implications. Multipoint calibration identified model structural adequacy and led to refinements in ATS including a more observation-consistent subsurface model and improved snow representation. Projections of permafrost thaw through the end of this century subjected to calibration-constrained soil property uncertainty indicated a factor of 3 increase in active layer thickness (maximum annual thaw depth). Comparisons of the effect of soil property uncertainty to climate model selection uncertainty indicated that while soil properties are a significant contributor to permafrost thaw projection uncertainty, climate model selection uncertainty is larger. We quantified the relative affect of three dominant environmental conditions, organic layer thickness, snowdepth, and amount of water on the landscape. Furthermore, sensitivity analysis using ATS identified the canceling effects of interaction between increased latent heat demand and thermal conductivity due to variable saturation.

Given these advances in NGEE Arctic Phase 1, we look forward to coming work in Phase 2, especially continuing efforts to incorporate NGEE field data into fine-scale models. We will describe the integration of geophysical forward modeling into ATS, focused on the integration of electrical resistivity tomography (ERT) surveys with ATS hydrothermal simulations. The results of this work will be a joint inversion framework for coupling ERT surveys and ATS simulations. Similarly, models are being evaluated using the Barrow tracer experiment to gain understanding of the role of lateral flow within a polygon. And finally, we will discuss plans for Seward Peninsula models as NGEE Arctic moves to this new field site.

Implementing a Shared Project Management Strategy across NGEE-Arctic and NGEE-Tropics

Susan Heinz¹, Sandy Chin², Lara Kueppers², Jeff Chambers², and Stan Wullschleger¹

¹Oak Ridge National Laboratory, Oak Ridge, TN, United States

²Lawrence Berkeley National Laboratory, Berkeley, CA, United States

The NGEE-Arctic and NGEE-Tropics projects are major research efforts working to achieve – each in different terrestrial ecosystems – improved prediction of climate through knowledge derived from model-inspired studies in the field and laboratory. Both projects are composed of interdisciplinary teams collaborating across multiple national laboratories and institutions on a number of challenging and innovative science objectives. Given the complex and multi-institutional nature of NGEE research, strong science leadership and project management are of critical importance to ensure successful coordination of researchers, execution of tasks, and delivery on objectives. As such, NGEE-Arctic and NGEE-Tropics are working together to implement a common project management strategy that allows each to effectively manage team communications, information sharing, task and deliverables management, and to track performance and progress against a set of defined metrics.

Traditional project management methodologies are geared toward projects in which solutions and requirements are rigidly defined, large changes in scope are not expected, and tasks are routine and repeatable. Cutting-edge science research programs, however, require an approach of flexibility and agility because deliverables are novel, iterative and may transpire over the course of years. It is a significant challenge for researchers, project staff, managers and stakeholders to confidently address a constant flux environment of risk and change while showing progress on project vision and goals.

As one component of meeting these challenges, the collaboration software **Teamwork Projects** is being adopted to provide a comprehensive project management framework for identifying and tracking tasks, setting milestones, sharing documents and information, and following progress within a collaborative environment that allows for project transparency in the following ways:

- Provides clarity into work processes (i.e., who is doing what, when, where)
- Facilitates discussions between interdependent teams
- Team members are empowered to document their progress and issues
- Supports the sharing of “tacit knowledge” that may otherwise remain with individuals
- Supports team understanding and focus on the big picture – project goals and vision
- Allows management to monitor and respond readily to change

Although early in the process, the collaboration software also looks to provide the opportunity to track and collect useful metrics for a common dashboard reporting to sponsors from the two projects.

Abstract submission for the DOE TES and SBR Programs' ESS PI Meeting

Program: Terrestrial Ecosystem Science (TES)

PI: Stan Wullschleger

Title: The NGEA Arctic Data Archive: Data Sharing, DOI Services, and Modeling Archive

Authors: Terri Killeffer², Les Hook¹, Ranjeet Devarakonda¹, Misha Krassovski¹, Michael Crow¹, and Tom Boden¹

Author Affiliation: ¹ Environmental Sciences Division, ORNL and ²Information International Associates, Oak Ridge, TN

Email address: killefferts@ornl.gov; hookla@ornl.gov; devarakondar@ornl.gov; krassovskimb@ornl.gov; crowmc@ornl.gov; bodenta@ornl.gov

Abstract:

The Next-Generation Ecosystem Experiment (NGEE) Arctic project is composed of an array of researchers and disciplines across multiple national laboratories and universities. Project-generated datasets will improve representation of complex interactions of arctic land surface and subsurface processes in Earth System Models (ESMs). Because of the iterative approach of modelers, researchers are encouraged to share their data early and often for use and input into research needs. The NGEA Arctic Data Management Team (DMT) at ORNL, with assistance from Data Representatives at each collaborating institution, are charged with collecting, archiving and sharing data within the project, the larger scientific community, and the public. Access data at the NGEA Arctic home page [<http://ngee-arctic.ornl.gov>] and click "Search Data." Moving forward into Phase 2 of the project, the DMT would like to present several areas of focus:

Data Sharing Metrics

To track data sharing progress, we developed metrics for the number of metadata records available, planned datasets, datasets available to the project or public, and number of data downloads. The project is striving to meet the DOE Office of Science Statement on Digital Data Management requiring data that supports or validates research results in a publication are published at the same time the paper is published.

DOI Services

All datasets intended for public sharing receive a Digital Object Identifier (DOI). Researchers are highly encouraged to request a DOI from the DMT early in dataset development so the DOI is available for inclusion in manuscripts submitted for review. We are beginning to track the associations of NGEA Arctic datasets in NGEA Arctic related publications and attempting to track in publications outside the project using NGEA Arctic data. We intend to share this cross-referencing of DOIs and publications with publishers to assist with their metrics as well as NGEA Arctic metrics of use and re-use of datasets.

Modeling Archive

In consultation with the NGEA Arctic Modeling Team, the DMT has developed an approach for archiving modeling products. The DMT is customizing the Metadata Entry and Data Upload Tool to assist in model archive submissions and the creation of landing pages. The landing page will include a DOI and citation for the modeling archive plus driver data, code, configuration documentation, model output, post-processing documentation, and condensed results (e.g., figures). The modeling archive provides documentation and reproducibility of model simulations that are being requested by journals and meet the aforementioned requirements of DOE.

Characterizing biotic and abiotic properties of landscape and their implications for ecohydrological processes across scales

Jitendra Kumar, Zachary L. Langford, Forrest M. Hoffman

Oak Ridge National Laboratory

Abstract

Ecohydrological processes governing the dynamics of terrestrial ecosystems and its response and feedback to climate change occur at diverse spatial and temporal scales. To accurately capture the dynamics of ecohydrological processes in the model, it is critically important to capture the subgrid scale heterogeneity of the landscape and develop scale aware process representation and parameterization. This study focused on the Arctic tundra landscape at Seward Peninsula of Alaska. Ecohydrological processes in this sensitive landscape are strongly governed by the physical and structural properties (like topography, soil, permafrost, geomorphology etc.) of the landscape, environmental conditions (like temperature, precipitation, light, radiation) and biotic conditions (vegetation, above/below ground biomass and organic matter, disturbance history etc.). From site to watershed to regional scales (scales at which models often operate), landscape is a complex mosaic of a range of biotic and abiotic properties. We have developed and applied a hierarchical characterization and classification approach to segment the landscape in distinct units which can be used to develop and parameterize process models at local scale. We also analyze how the distribution and organization of the landscape units as building blocks influence and interact with ecosystem processes across scales. Our goal is to understand the landscape organization principles and their roles to inform and improve process based models of ecohydrological processes in Arctic tundra landscape.

Contact: Jitendra Kumar (jkumar@climatemodeling.org)

Quantifying the Distribution of Soil and Permafrost Properties and Their Linkage with Landscape Properties in Arctic Tundra Ecosystem

Emmanuel Léger, Baptiste Dafflon, Haruko Wainwright, Yuxin Wu, Tim Kneafsey, John Peterson, Craig Ulrich, Jonathan Ajo-Franklin, Susan Hubbard

Lawrence Berkeley National Laboratory

Improving understanding of arctic ecosystem functioning and parameterization of process-rich models that simulate feedbacks to a changing climate require advances in estimating the spatial and temporal variations in land surface, active layer, ice-wedge and permafrost properties. In the context of the Next-Generation Ecosystem Experiments (NGEE-Arctic), we are developing advanced geophysical strategies to improve characterization and monitoring of Arctic ecosystems. An overarching objective is to develop methods that can bridge the wide gaps between the native scales where processes occur (typically <1m) and the scales needed to inform and validate models (typically >10s of kms). To meet this objective, we have performed laboratory and field geophysical efforts and have developed new geophysical acquisition, inversion and interpretation approaches. We are using a variety of acquisition strategies, including point measurements, ground-based measurements, and aerial platforms – some collected autonomously. Field investigations have been performed at the NGEE site, located in the Barrow Environmental Observatory (BEO) near Barrow (AK), which is dominated by different types of ice wedge polygons. Preliminary investigations are underway at two sites near Nome (AK), a warmer region compared to Barrow, with more topography and less continuous permafrost.

We describe the use of multi-dimensional relationships between physical and biogeochemical properties, developed at the lab scale and translated to the field scale. Examples include the estimation and mapping of soil organic matter density, ice-content and salinity informed by X-ray computed tomography and electrical resistivity tomography (ERT) data. In addition, Ground Penetrating Radar (GPR) and ERT methods have been successfully used for imaging thaw layer properties during the growing season and for estimating active layer thickness during the frozen season as well for delineating the geometry of permafrost features such as ice-wedges in Barrow. We are also developing two new research paradigms for characterization and monitoring associated with suites of properties or compartments important for system functioning. One is the development of new above-and-below ground geophysical monitoring approaches to illuminate the co-dynamics of ecosystems and critical bedrock-through-canopy interactions. The other is the development of a Bayesian approach for identifying functional zones in the landscape, which have unique distributions of property suites that are important for ecosystem functioning relative to neighboring regions. Together, the geophysics-based acquisition and inversion approaches are providing unique high-resolution information and new insights about the Arctic ecosystem functioning as well as providing information to models – at scales and resolutions useful for predicting terrestrial ecosystem feedbacks to the climate.

Understanding Lateral Hydrological Flow Paths in the Arctic Coastal Plain

Brent D. Newman¹, Jeffery M. Heikoop¹, Heather M. Throckmorton¹, Nathan A. Wales¹, Cathy J. Wilson¹, and Stan D. Wullschleger²

¹Earth and Environmental Sciences Division, Los Alamos National Laboratory, Los Alamos, NM USA; ²Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge TN, USA

This study examines lateral factors and processes critical to predicting the carbon-, nitrogen-, and water-balances of tundra ecosystems and will inform modeling efforts for predicting hydrologic and ecosystem responses with projected climate change and landscape evolution. Water and nutrient dynamics of tundra ecosystems are being studied as part of the DOE Next Generation Ecosystem Experiment (NGEE) Arctic project. This presentation synthesizes results from Phase I of the NGEE Arctic project in Barrow, Alaska (USA) and includes individual polygon-scale tracer testing as well as isotopic and geochemical indicators of lateral connectivity/transport. The tracer tests were implemented on separate high- and low-centered polygons with the Barrow Environmental Observatory (BEO) in July, 2015. A bromide solution was sprayed on the surface of the polygon centers. Radial arrays of rhizon soil water samplers were used to track tracer movement out to adjacent troughs at up to three depths within the active layer. Grab samples were also taken in troughs and ponded areas. Results to date suggest that most of the transport has been vertical within the shallower depths within the centers of the polygons. However, there has been some lateral transport to the troughs at the low-centered polygon, although this has been limited to just a few sample locations. Sampling will continue over the 2016 warm season. At the landscape scale we have collected isotopic and geochemical data from interlake polygonal areas, drained thaw lake basins, and key drainages. Results suggest that isotopic and geochemical variability increase with scale from the polygons in the BEO intensive area to the larger landscape scale. These results suggest it will be important to consider the effects of the thaw lake basins and drainages at Earth System Model grid scales.

Characterizing rooting depth distribution and nitrogen acquisition by dominant tundra plant species

Ingrid J. Slette, Colleen M. Iversen, Victoria L. Sloan, Joanne Childs, Richard J. Norby, Holly M. Vander Stel, and Stan D. Wullschlegel

Rooting depth distributions may be an important factor controlling competition for water and nutrients among plant species in Arctic tundra. Permafrost thaw and degradation resulting from climate warming may increase the thickness of the active soil layer and alter the vertical distribution of plant-available nutrients. Species with root distributions that provide better access to nutrients in an altered soil profile may gain a competitive advantage. However, our ability to predict how tundra plant communities will respond to such changes is hindered by the fact that little is known about the rooting depth distributions and nutrient acquisition strategies of the dominant plant species in tundra ecosystems.

In July 2013, we conducted a ^{15}N isotope tracer experiment to assess the vertical distribution of soil nutrient acquisition among three dominant species representing important plant functional types on the Barrow Environmental Observatory in northern Alaska. We injected a solution of $^{15}\text{NH}_4\text{Cl}$ into the soil in either the organic horizon (3 cm), the mineral horizon (10 cm), or at the permafrost boundary (~ 30 cm), beneath 9×9 cm plots located in homogeneous patches of *Carex aquatilis* (sedge), *Eriophorum angustifolium* (sedge), and *Salix rotundifolia* (deciduous shrub). One week later, soil cores and aboveground vegetation were harvested from the plots. Aboveground leaf and stem biomass and the vertical distribution of root biomass were measured. Soil organic matter and above- and belowground plant tissues were analyzed for ^{15}N content.

Vertical patterns of root distribution and nutrient acquisition varied among the plant species. Both sedge species acquired substantially more ^{15}N from the mineral soil layer than from the organic soil layer, whereas the shrub acquired ^{15}N primarily from the organic soil layer. None of these species acquired much ^{15}N from near the permafrost boundary. The roots of the shrub were located almost exclusively in the organic horizon, which is consistent with the patterns of nutrient acquisition for this species. Contrastingly, the roots of the sedges extended throughout the soil profile, suggesting that root density does not entirely explain the patterns of nutrient acquisition for these species. Minimal plant ^{15}N uptake from near the permafrost boundary may limit the impact of climate warming-induced nutrient release from previously frozen soils. Results from this experiment are being used to improve model representations of tundra root dynamics and plant-soil interactions.

Next-Generation Ecosystems Experiment (NGEE Arctic): Progress and Plans

Stan Wullschleger, Tom Boden, Robert Bolton, David Graham, Susan Hubbard, Colleen Iversen, Alistair Rogers, Vladimir Romanovsky, Joel Rowland, Peter Thornton, Margaret Torn, William Riley, and Cathy Wilson

Oak Ridge National Laboratory, Oak Ridge, TN, United States

Los Alamos National Laboratory, Los Alamos, NM, United States

Lawrence Berkeley National Laboratory, Berkeley, CA, United States

Brookhaven National Laboratory, Upton, NY, United States

University of Alaska, Fairbanks, AK, United States

An important challenge for Earth System Models (ESMs) is to accurately represent land surface and subsurface processes and their complex interactions in a warming climate. This is true for all regions of the world, but it is especially important for high-latitude Arctic ecosystems which are projected to warm at a rate twice that of the global average by the end of the 21st century. The Next-Generation Ecosystem Experiments (NGEE Arctic) is a 10-year project (2012 to 2022) that seeks to increase our confidence in global climate projections through a coordinated series of model-inspired investigations undertaken by a collaborative team of modelers, data managers, and empiricists spanning a range of scientific disciplines. NGEE Arctic focuses on high-latitude ecosystems underlain by carbon-rich permafrost that are vulnerable to thaw in a warmer climate. In Phase 1 (2012 to 2014), NGEE Arctic tested and applied a multi-scale measurement and modeling framework for ecosystems and watersheds characterized by cold, continuous permafrost on the North Slope of Alaska. These efforts provided datasets for model parameterization and benchmarking and knowledge on topics ranging from watershed hydrology to plant physiology. These data are being adopted by DOE's Earth System Modeling program as fundamental new developments in a next-generation ESM, the Accelerated Climate Model for Energy (ACME). In Phase 2 (2015 to 2018), we have established a southern field site on the Seward Peninsula which, compared to our research site on the North Slope, is characterized by transitional ecosystems; warm, discontinuous permafrost; higher annual precipitation; and well-defined watersheds with strong topographic gradients. Our selection of the Seward Peninsula is based on a Phase 1 analysis indicating that western Alaska is a proxy for the future ecological and climatic regime of the North Slope of Alaska toward the end of the century. New sites on the Seward Peninsula will expand our understanding and model representation of (1) landscape structure on the storage and flux of carbon, water, and nutrients, (2) edaphic and geochemical mechanisms responsible for variable CO₂ and CH₄ fluxes across a range of permafrost conditions, (3) variation in plant functional traits across space and time, and in response to changing environmental conditions, (4) controls on shrub distribution and associated climate biogeochemical and biophysical feedbacks to climate, and (5) changes in surface and groundwater hydrology expected with warming in the 21st century. Our vision in Phase 1, and now extended into Phase 2, strengthens the connection between process studies in Arctic ecosystems and high-resolution landscape modeling and scaling strategies that will foster a strong interaction across the DOE Biological and Environmental Research (BER) program. The NGEE Arctic project supports the BER mission to advance a robust predictive understanding of Earth's climate and environmental systems by delivering a process-rich ecosystem model, extending from bedrock to the top of the vegetative canopy/atmospheric interface, in which the evolution of Arctic ecosystems in a changing climate can be modeled at the scale of a high-resolution, next-generation ESM grid cell. Research in Phase 1, and now proposed for Phase 2, prepares our team for pan-Arctic simulations of ecosystem-climate feedbacks in Phase 3 (2019 to 2022). Safety, collaboration, communication and outreach, and a strong commitment to data management, sharing, and archiving are key underpinnings of our model-inspired research in the Arctic.

Influences of climate warming on labile organic carbon transformation and mercury methylation in saturated tundra from Barrow, Alaska

Ziming Yang^{1*}, Stan D. Wullschleger^{1,2}, Liyuan Liang¹, David E. Graham^{2,3}, Baohua Gu¹

Terrestrial Ecosystem Science Program: NGEE-Arctic Project (PI: Stan D. Wullschleger)

¹ Environmental Sciences Division, Oak Ridge National Laboratory

² Climate Change Science Institute, Oak Ridge National Laboratory

³ Biosciences Division, Oak Ridge National Laboratory

* Corresponding author email: yangz1@ornl.gov

Warming temperatures in Arctic tundra increase microbial activity and thus stimulate the degradation of stored soil organic carbon (SOC). Previous studies suggest that SOC degradation is affected by its chemical composition, but it remains unclear what fractions or pools of SOC are the most vulnerable to rapid breakdown and what mechanisms are involved. Additionally, little is known concerning the effects of permafrost thaw on microbial mercury methylation and how it is coupled to SOC degradation. Using a suite of analytical techniques, we examined the dynamic consumption and production of labile SOC compounds, including reducing sugars, alcohols, and low-molecular-weight organic acids during an 8-month anoxic incubation with a tundra soil obtained from the Barrow Environmental Observatory, Barrow, Alaska. We observe that sugars and alcohols in thawed SOC largely account for the initial rapid release of CO₂ and CH₄ through anaerobic fermentation; organic acid fermentation products are subsequently utilized as substrates for methanogenesis. Degradation of labile SOC is also found to rapidly fuel the biosynthesis of methylmercury, a potent neurotoxin in tundra soil. Mercury methylation is positively correlated to the production of CH₄ and ferrous ion, suggesting the linkages among microbial pathways of methanogenesis, iron reduction, and mercury methylation. These observations suggest that climate warming or permafrost thaw could greatly enhance the decomposition of labile SOC, which accelerates the release of CH₄ and CO₂ and production of methylmercury in Arctic tundra.

Linkage between root competitive traits and tundra nitrogen uptake patterns

Abstract

The Arctic tundra carbon dynamics are strongly limited by nitrogen availability, due to slow mineralization, slow nitrogen fixation, and trivial nitrogen deposition. Ongoing climate warming will likely perturb vertical distributions of nitrogen availability in tundra ecosystems through enhancing nitrogen mineralization and releasing frozen nitrogen from permafrost soil. However, arctic tundra responses to such changes are unclear, because of both the lack of vertically explicit nitrogen perturbation field experiments and untested hypotheses of root nitrogen uptake implemented in land models. In contrast to N uptake data in other ecosystems (*e.g.*, grasslands, agro-ecosystems), our vertically explicit ^{15}N tracer experiment (for three dominant tundra species: *Carex aquatilis*, *Eriophorum angustifolium*, and *Salix rotundifolia*) showed that plant nitrogen uptake profiles were not consistently related to profiles of soil available nitrogen or root biomass density. These results challenge both the prevailing hypothesis that root density always exerts first order control on nitrogen uptake and the model structures that apply this hypothesis. Applying a recently developed model of nutrient competition based on the Equilibrium Chemistry Approximation (ECA), we explained the paradoxical observations with: (1) highly competitive but shallow rooting plant species that obtain most of their nitrogen from topsoil under the stress of microbial nutrient competition and (2) poorly competitive species that absorb more nitrogen from deeper mineral soils, where microbial nutrient demand is low. Sensitivity analyses revealed that plant nutrient affinity (a proxy for competitiveness) could surpass the effect of root biomass density and exert a first-order control on nitrogen uptake patterns. Currently applied methods to resolve nutrient competition (*e.g.*, relative demand, microbes outcompete plants) were unable to explain the diversity of observed plant N uptake profiles. Our results (1) cast doubt on current climate-scale model predictions of arctic plant responses to elevated nitrogen supply under changing climate and (2) highlight the importance of considering essential root functional traits in large-scale Earth System Models (ESMs).

NGEE TROPICS ABSTRACTS

NGEE-Tropics Overview Abstract

Tropical forests cycle more CO₂ and water than any other biome, and are critical to Earth's energy balance. Yet processes controlling tropical forest carbon cycling are not well established, and large uncertainties in observational estimates and Earth system model (ESM) projections of net carbon fluxes remain unresolved, contributing significant uncertainty to climate projections. Thus the overarching goal of NGEE-Tropics is to develop a predictive understanding of how tropical forest carbon balance and climate system feedbacks will respond to changing environmental drivers over the 21st Century. To accomplish this goal, NGEE-Tropics will develop a transformational, process-rich model framework where the evolution and feedbacks of tropical forests to a changing climate are modeled at the scale of a next generation ESM grid cell. Research in Phase 1 will develop improved understanding and model representation of key tropical forest processes including: responses to changing temperature, precipitation, and atmospheric CO₂; disturbance and land-use change; and heterogeneity in belowground processes. Model development and measurement activities will be integrated at pilot study field sites. A data synthesis and management framework will be developed to build and provide data products via a community portal. Phase 1 will provide a foundation for research on pantropical forest interactions with climate for NGEE-Tropics Phases 2 and 3.

From leaf to ecosystem level: controls of transpiration in seasonal tropical forests across a rainfall gradient

Matteo Detto, Brett Wolfe, Helene Muller-Landau Joseph Wright and Stuart Davies

Introduction

The role of environmental drivers in regulating gas exchange in tropical forests are still poorly understood. This inhibits the development of Earth System models that project responses to future climate scenarios. In order to better understand the responses of plants to climatic variation we need high quality environmental measurements in conjunction with plant physiological measurements on a broad range of temporal and spatial scales, which span leaf to ecosystem levels and climate gradients.

Central American moist tropical forests are characterized by a distinct dry season and a rainfall gradient, where the Pacific is drier than the Atlantic side. This normal seasonal cycle is often altered during ENSO events, which generally produce large interannual variability and warm/dry conditions over this part of the tropics.

We take advantage of this climatic gradient and a strong ENSO event to assess how plant transpiration responds to environmental drivers.

Experiment description

The three experimental sites, Parque Natural Metropolitano (PNM), Barro Colorado Island (BCI) and San Lorenzo National Park (SLZ), were located in central Panama across a rainfall gradient. Principal meteorological variables (solar radiation, air temperature, relative humidity) and soil moisture were monitored by automated stations. In addition, at BCI, a microclimatic station equipped with an eddy covariance system measured energy and CO₂/H₂O fluxes starting from 2012. Plant level measurements, starting from November 2015, included automated sapflow and canopy temperature. Periodically, through access with canopy cranes, leaf water potential and leaf gas exchange were measured.

Preliminary results

The climate in this region is characterized by a distinct dry season from mid-December to April, when soil moisture dropped quickly. At the same time, atmospheric demand of water increased, because of higher solar radiation from reduced cloud cover, lower relative humidity and sustained winds. In the wet season, direct radiation declined sensibly, but the diffuse component remained approximatively constant.

Ecosystem scale evapotranspiration, measured by the eddy covariance system, showed that water losses were approximatively constant across the year, despite increased atmospheric demand in the dry season. This may indicate stomatal control is active during the dry season to avoid excess water losses. Similar results were shown by sapflow measurements. However, sapflow exhibited high interspecific variability, with some species responding differently to environmental stimuli.

Across the rainfall gradient, large differences were observed in canopy temperature, where the dry site (PNM) showed higher temperature in the day and larger diurnal fluctuation.

A large community of scientists are now working on the inclusion of vegetation demographic models (VDMs) in Earth System Models. These developments are a clear opportunity to increase the fidelity of how ecosystem are represented in ESM's. They also pose a huge challenge, owing to the increased model complexity and the new potential for model-data interaction which they provide.

Challenges collectively faced by this community include parameterization in very high-dimensional space, initialization of vegetation structure, understanding complex internal feedback processes, the representation of co-existence, and the availability and usefulness of benchmarking and validation data. Underpinning these emergent properties of VDMs are a set of additional process representations, distinct from those in traditional land surface models, which together allow ecological dynamics to be simulated, but also add an additional dimension of process uncertainty. Here we collate progress so far on the inclusion of VDMs in ESMs, assess the new model features necessitated by these development, consider alternative model formulations and opportunities for progress. Finally, we assess driver and benchmarking datasets; those that are available, and observational gaps specific to VDMs which are so far poorly constrained.

Forecasting Pan-Tropical Ecological Impacts of the 2015 El Niño Southern Oscillation (ENSO)

Forrest M. Hoffman*¹ and Min Xu¹

¹Oak Ridge National Laboratory, Oak Ridge, TN, USA

February 26, 2016

The El Niño Southern Oscillation (ENSO) is an irregular periodic climate fluctuation, occurring every eight to 12 years, that is driven by variations in sea surface temperatures (SSTs) over the tropical eastern Pacific Ocean and extending westward across the equatorial Pacific. The warming phase is called El Niño and the cooling phase is called La Niña. This dominant ocean cycle, linked with the Walker Circulation, affects ocean turnover and nutrient availability, as well as temperatures and precipitation globally. El Niño also has strong effects on the global carbon cycle seasonally because, although weakened ocean circulation reduces marine carbon outflow, terrestrial emissions more than compensate for this reduction. Strong drying conditions in the Asia-Pacific region and western South America during El Niño lead to reduced ecosystem productivity and increased mortality and fire risk, which are responsible for the increased source of carbon to the atmosphere.

A record-setting El Niño appears to be setting up for a late fall or early winter peak, providing relief from the California drought but portending hot and dry conditions for the island nations of the western Pacific. To study the responses and feedbacks of drought effects induced by ENSO events, we have conducted a series of global Earth system model simulations using the Accelerated Climate Model for Energy (ACME) v0.3 model. These simulations will draw upon the ensemble of NOAA ENSO forecast sea surface temperature (SST) predictions that extend 9 months into the future. The experimental design consists of a carbon cycle spin up simulation using repeated 1982–2006 SST forcing from reanalysis, 5-y ENSO simulations for the 1997 (1996–2000) and the 2015 (2014–2018) events, and one or more non-ENSO control simulations. A combined set of historical and NOAA forecast SSTs are being used for the 2015 ENSO simulations. Analysis of ecosystem impacts, investigating anomalies in soil moisture, GPP, and stomatal conductance, will be performed across both events. ACME coupler output from the atmosphere will be saved at 3- or 6-h frequency for use as offline forcing for new model parameterization development and testing within the NGEE Tropics project.

*Corresponding author e-mail address: forrest@climatemodeling.org

Linking ecosystem demography modeling and field experiments to understand tropical forest response to novel disturbance regimes

Jennifer A. Holm¹, Charles D. Koven¹, Rosie A. Fisher², Ryan G. Knox¹, Robinson I. Negrón-Juárez¹, Jeffrey Q. Chambers^{1,3}, Daniel Magnabosco Marra^{4,5,6}, Sami W. Rifai⁷, Niro Higuchi⁶, Lara Kueppers¹

¹ Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, CA 94720, USA

² National Center for Atmospheric Research, Boulder, CO 80301, USA

³ Department of Geography, University of California, Berkeley, Berkeley, CA 94720, USA

⁴ Institute of Biology, University of Leipzig, Johannisallee 21 04103 Leipzig, Germany

⁵ Max Planck Institute for Biogeochemistry, Jena, Germany

⁶ Brazil's National Institute for Amazonian Research, Manaus -AM, Brazil

⁷ School of Forest Resources and Conservation, University of Florida, Gainesville, FL 32603, USA

ESS PI Meeting Abstract:

Changing climates and disturbance regimes of the 21st Century will push tropical ecosystems into novel states that have no-analog in the recent historical record. In addition, inaccurate simulations of tropical forests contributes to multiple biases in Earth System Models (ESMs) and results in disagreement among models regarding whether tropical forests will be future carbon sources or sinks. Vegetation demography, plant competition among tree size classes, mechanistic mortality, and plant functional traits strongly control carbon dynamics and energy budgets of the Earth's surface. These processes have not been represented in the widely used Community Land Model (CLM) until the recent inclusion of the Ecosystem Demography (ED) model into CLM 4.5, i.e., CLM-ED, which is the base model for further development in the NGEE-Tropics Project. The goal of this study was to compare ecosystem demography model predictions to field measurements across gradients in tropical carbon cycling and community composition in Amazonia. Models include a dynamic, individual-based demographic gap model, ZELIG-TROP, and the Ecosystem Demography v.2 (ED2) and CLM-ED dynamic vegetation models. Field measurements were used to generate both model parameterization and benchmarking datasets for the Amazon Basin as a whole, and the northwest Amazon (NWA) and the Central Amazon (CA) separately.

When comparing models of different scales, CLM-ED over-estimated biomass in the >100 cm size class by 90+ Mg ha⁻¹, thus largely overestimating aboveground biomass, and over predicts growth and mortality rates compared to field data. ED2 underestimated the aboveground biomass stock (231 vs. 312 Mg ha⁻¹) for a CA forest, and similar to CLM-ED exhibits fast growth and mortality rates leading to an over prediction of the Central Amazon carbon sink. Model validations of ZELIG-TROP confirmed that the NWA and CA simulations successfully reproduced observed values of net primary productivity, biomass, and leaf area index, and mortality rates, but predicted slightly lower growth rates. Modeling the existing tree mortality gradients across Amazonia is a complex task, yet essential to reliable prediction of carbon storage in a warmer climate. Using ZELIG-TROP, we evaluated the response of Amazonian forests to elevated mortality rates. The simulated NWA with doubled mortality rates (from 2% to 4%) was found to have a significant decrease in biomass (29.6%) and a slight decrease in NPP compared to a control simulation. However, there was a non-significant shift in community composition in the NWA forests (Wilcoxon rank sum, Z=0.95, p=0.34). When mortality was doubled in the CA significant changes in basal area and community composition were observed (Z=2.28, p=0.02) but this shift did not generate a community composition representative of the observed NWA. Our modeling results suggest that species composition in CA is more sensitive to a doubling of mortality rates than in NWA leading to a larger decrease in biomass in CA (41.9%).

Disentangling temperature-driven influences to water and carbon plant physiological processes in the Central Amazon during the 2015/16 El Niño

Kolby J. Jardine, Jennifer Holm, Robinson Negrón-Juarez, Angela B. Jardine, Clarissa G. Fontes, Bruno Gimenez, Todd E. Dawson, Thomas Powell, Jeff Chambers, and Niro Higuchi

Tropical forests cycle more carbon and water than any other terrestrial biome, but are highly sensitive to warming climates. Improvement of terrestrial carbon and water cycling predictions requires a better understanding of the physiological mechanisms underlying forest response to warming. The 2015/6 drought associated with El Niño in the Amazon Basin offered a unique opportunity to collect coupled field observations of plant physiological and environmental variables which are indicated by models to be the most critical for predicting the future of tropical forest carbon, water, and energy fluxes. Observations from the Central Amazon have found leaf temperature to strongly control both water and carbon plant physiological processes. In situ measurements of net photosynthesis and stomatal conductance peaked in the morning and showed a clear mid-day/post-midday depression associated with temperatures passing the optimal value for net photosynthesis ($\sim 32^\circ\text{C}$). Despite assumptions of a significant time delay, tight temporal correlations were found between sap velocity (1m) and crown leaf temperature. Leaf water potential (Ψ_L), which reflects the balance between sap flow and transpiration, is assumed to reach a minimum during mid-day. However, in-situ observations show that despite high leaf temperatures, dramatic recoveries (20-70%) in Ψ_L occur around mid-day in Central Amazonian trees, potentially due to an increase in the sap flow/transpiration ratio influenced by both a decrease of stomatal conductance after 10:00 am and the strong coupling of sap flow with leaf temperature. Additionally, plant monoterpenes protect photosynthesis during high temperature stress, but little is known about the composition of monoterpenes in tropical ecosystems. Here we show that monoterpene emissions from leaves are linked with recent photosynthesis and demonstrate distinct temperature optima for five monoterpene groups, potentially corresponding to different enzymatic reaction pathways within the β -ocimene synthase family. As temperatures increased during the 2015 El Niño in the Central Amazon, diurnal and seasonal leaf and ecosystem emissions showed strong linear increases in the relative abundance of linear β -ocimenes ($+4.4\% \text{ } ^\circ\text{C}^{-1}$) at the expense of cyclic and bicyclic isomers (e.g d-limonene and α -pinene, respectively). The negative temperature sensitivity of α -pinene, currently assumed to dominate tropical monoterpene emissions, could not be reproduced using current global emission models. Given that β -ocimenes are highly reactive with respect to atmospheric and biological oxidants, these observations suggest a functional role at high temperatures through cloud condensation nuclei formation and within-plant antioxidant roles. The results demonstrate a strong coupling of sap flow and leaf temperature and demonstrate monoterpene emission composition as a new highly relevant signal for warming impacts on tropical terrestrial carbon cycling in future studies.

Modeling hydrologic processes in the Amazon: Comparison of hydrologic variability in a hierarchy of model simulations

Ruby Leung, Ethan Coon, Zhuoran Duan, Yilin Fang, Pieter Hazenberg, Hongyi Li, Jie Niu, Scott Painter, William Riley, Chaopeng Shen, Mark Wigmosta, Xubin Zeng

Water is essential for plants, which obtain most of their water through soil water uptake. Understanding and modeling the spatial and temporal variability of surface and subsurface water available to plants is thus essential for predicting how tropical forests will respond to climate change. Although hydrological processes may be reasonably well represented in models at their native spatial and temporal scales, significant challenges remain in rendering the effects of those processes at climate-relevant scales. Systematic benchmarking and process-based evaluation of key processes important for tropical forest may provide expedient ways of improving hydrologic modeling in Earth System Models. As part of the NGEE Tropics project, hydrologic modeling experiments have been designed to identify preferable modeling alternatives that can be readily adopted by Earth System Models for improving representations of surface and subsurface hydrology and identify remaining model development needs. In the first of a series of numerical experiments, simulations are performed over the Asu catchment in the Amazon where soil moisture, groundwater level and stream gauge measurements are available for model evaluation. A hierarchy of one-dimensional to three-dimensional models including the ACME Land Model (ALM), DHSVM, CLM-PAWS, CLM-ParFlow, CLM-PFLOTRAN, Amanzi/ATS, and h3D are applied to simulate hydrologic variability from hourly to interannual time scales. Preliminary results will be presented, with initial focus on seasonal and interannual variability, particularly contrasting the hydrologic response simulated by different models between wet and dry years.

NGEE-Tropics El Nino and drought impacts research

Arguably the largest threat to the tropical carbon sink is drought, via reductions in carbon uptake and increases in turnover. The 2015-16 El Nino event caused pan-tropical drought manifest as reduced precipitation and elevated temperature. Through NGEE-Tropics we are quantifying the impacts of this recent drought on many aspects of vegetation stress and using these data to inform us regarding processes and to improve model representation of tropical forest drought resistance.

Photosynthetic parameters of diverse woody species in Panama are correlated with foliar nitrogen and phosphorus content

Richard J. Norby¹, Lianhong Gu¹, Ivan Haworth¹, Ben Turner², Anthony Walker¹, Jeffrey M. Warren¹, David Weston¹, Klaus Winter², and Joe Wright²

¹Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN, USA; ²Smithsonian Tropical Research Institute, Panama

Phosphorus (P) availability exerts a strong control on the productivity of lowland tropical forests. However, the observed variation in productivity across P gradients is poorly represented in terrestrial biosphere and Earth system models because the models lack routines to estimate P availability and its influence on productivity. While detailed biogeochemical models of P availability are currently being developed, the physiological effect of phosphorus limitation is often represented as a stoichiometric downscaling of GPP, if it is included at all. To inform the development of a physiological model of P limitation, we developed empirical relationships between foliar P content and photosynthetic parameters for tropical trees in Panama. We measured the A-Ci relationship in upper canopy leaves of about 90 woody species at two locations differing in soil fertility and floristic composition. Measurements with LiCor 6400 systems were made from canopy cranes in a seasonally dry forest, Parque Natural Metropolitano near Panama City, and a moist forest, Parque Nacional San Lorenzo near Colon. After determination of leaf area and dry mass, leaves were analyzed for nitrogen (N) and P content at the Smithsonian Tropical Research Institute.

Foliar C:N:P ratios varied widely across species, with N:P ratios ranging from 7 to 42, suggesting that some trees may have been N-limited, some P-limited, and many co-limited by N and P. V_{cmax} , J_{max} , and TPU were correlated with both leaf P and N contents across all species; all relationships were stronger when nutrient contents were expressed on a leaf area basis. From a multivariate perspective the best expression of photosynthetic traits predicted J_{max} from both N and P, with V_{cmax} predicted in relation to J_{max} . Nutrient contents and photosynthetic parameters were significantly less at the more nutrient-poor San Lorenzo site, but trees from both sites could be described by the same relationships. Although all of the species measured in this study are classified as the same plant functional type (broadleaf tropical evergreen) in most models, they were taxonomically and functionally diverse. Models may be more accurate if this PFT could be defined more narrowly with nutrient and photosynthetic parameters specific to a well-defined subgroup. However, variation in photosynthetic parameters among species was unrelated to phylogenetic position. Wood density, which may be a surrogate measure of growth rate or successional status, was a significant predictor of J_{max} , strengthening the relationship with N and P for a subset of plants for which wood density data were available. Trait covariance may be a useful approach for improving physiological expressions of photosynthesis in nutrient enabled models.

Development and management of tropical forest datasets for model simulation and benchmarking

Charuleka Varadharajan, Gilberto Pastorello, Danielle S. Christianson, Boris Faybishenko, Ping Hu, Ranjeet Devarakonda, Michael Crow, Terri Killeffer, Les Hook, Tom Boden, and Deb Agarwal

New and existing ecological, hydrological, and meteorological datasets from tropical forests in Central and South America are being collected and utilized in the U.S. Department of Energy's NGEE Tropics project. One of the primary goals of the NGEE Tropics data team is to enable efficient generation of data synthesis and analysis products for the project in a repeatable and scalable manner, by developing an agile infrastructure. Currently components of the infrastructure have been developed to standardize data and metadata collection activities, archive NGEE Tropics datasets, and provide data for model parameterization.

We have developed standardized templates to report metadata for various field measurements by working with the data collectors. The objective was to minimize effort required to archive a dataset, while maximizing the utility of search and synthesis across datasets. Metadata specifications were based on project data collection protocols, example data files submitted, and other related protocols, e.g., Smithsonian Tropical Research Institute (STRI) and AmeriFlux. We have built the NGEE Tropics Archive, an accessible and searchable repository, to host all data generated in the project, including field measurements, simulation results, and data products. The Archive leverages the NGEE Arctic data management system and complies with DOE Office of Science Digital Data Management Requirements. Data files generated in a common theme, such as an experiment, field campaign, data synthesis product, or a publication, will be grouped into collections for submission to the archive. Data collections will be archived following basic QA/QC checks, documentation, assignment of a DOI, and will be made available to the project team and public.

High priority datasets from the Archive will receive additional QA/QC, processing, and transformations. For example, in partnership with the modeling team and the data provider—STRI, we conducted QA/QC processing of meteorological data from Barro Colorado Island, Panama, to provide input parameters for numerical simulations using climate models. This involved gap-filling of missing data, removal of outliers, and flagging of suspicious segments of the time series, which allowed us to create a consistent dataset of meteorological drivers.

In the future, access to NGEE Tropics and other community data will be available through a data broker and web portal that will provide an integrated data search, visualization, analysis, and access interface. The underlying infrastructure is being developed to meet project needs to perform specific data queries, create synthesis products, initiate automated QA/QC, and transform data for model parameterization and benchmarking tasks.

UNIVERSITY - SBR ABSTRACTS

Evaluating Trace Metal Limitations on Methane Fluxes in Terrestrial Ecosystems

J.G. Catalano (PI, catalano@wustl.edu), A.S. Bradley, N.M. Crompton, D.E. Giammar—*Washington University in St. Louis*; L.G. Chambers—*University of Central Florida*; E.A. Hasenmueller—*Saint Louis University*

Supported by the Subsurface Biogeochemical Research (SBR) Program

The greenhouse gas methane (CH₄) is produced in terrestrial ecosystems by subsurface microbial carbon cycling under anaerobic conditions. Its formation is localized at terrestrial-aquatic interfaces such as wetlands, permafrost soils, and soil microenvironments where oxygen is limited and organic carbon is available. Global climate models predict higher CH₄ emissions from wetlands in the future because of an increase in inundated area and the enhancement of CH₄ production as temperature increases. The large radiative forcing induced by increasing atmospheric CH₄ concentrations makes it critical to understand the environmental controls on CH₄ production.

Global models of methane biogeochemistry assess CH₄ fluxes at the grid cell level by accounting for microbial respiration rates and how these rates are affected by temperature, pH, and soil redox state. Temperature is a major control on CH₄ production, and recent work has shown that methanogenesis in terrestrial ecosystems displays a high activation energy, indicating that increasing temperature will result in a substantial increase in CH₄ emissions from wetlands. However, it has also been shown that this relationship over predicts the temperature response of CH₄ production in many systems, suggesting that other substantial limitations on methanogenesis are present. A potentially important limitation that has been largely overlooked is trace metal availability. Methanogens are unique in having high enzymatic requirements for trace metals (e.g., Ni, Co, Zn, and Mo). Laboratory studies, primarily involving pure cultures of methanogens or anaerobic bioreactors, have shown that limited availability of trace metals inhibits methanogenesis, but such limitations have not been investigated in the field.

We hypothesize that trace metal limitations are important controls on CH₄ fluxes in terrestrial ecosystems. To test this hypothesis, we have characterized the properties, CH₄ production potential, and speciation of trace metals in wetland soils from field sites in Missouri and Florida. Surface waters in these wetlands are low in trace metals, typically <0.05 μM, well below the 1 to 5 μM concentrations shown as optimal for methanogenesis in pure culture studies. Regional river waters and groundwaters, potential water sources for the wetlands, show similar suboptimal dissolved metal concentration. Initial microcosm studies reveal that the wetland soils from our sites show methanogenic activity when maintained under anoxic conditions. Assays of lipid biomarkers indicate the presence of substantial bacterial and archaeal communities, including marker indicative of methanogens. Solid phase characterization reveals trace metal concentrations in the soils on the order of 1 to 10 μg/g. Spectroscopic studies suggest that the native metal content is largely associated with minor detrital components (e.g., silicate minerals). Soils from both locations show a substantial binding capacity for metals that maintains low dissolved concentrations (<0.05 μM) except upon addition of exceptional metal loads. Soils from the Missouri site have greater binding capacity, and spectroscopic measurements show that metals added to these soils bind to thiol groups on organic matter. Binding occurs primarily to carboxylate groups in the Florida soil, accounting for its lower capacity for metals. These initial studies indicate that trace metal availability in the wetlands systems under investigation is far below optimal levels and suggests that methanogenesis at these sites may be trace metal limited.

A multiscale approach to modeling carbon cycling within a high-elevation watershed

Kate Maher¹, Matthew J. Winnick¹, Yuchen Liu², Jennifer L. Druhan², Corey R. Lawrence³, Reed Maxwell⁴, Carl I. Steefel⁵, Kenneth H. Williams⁵, Rosemary Carroll⁶

1. *Department of Geological Sciences, Stanford University, Stanford, California 94305, USA*
2. *Department of Geology, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA*
3. *U.S. Geological Survey, Denver, Colorado 80225, USA*
4. *Geology and Geological Engineering, Colorado School of Mines, Golden, Colorado 80401, USA*
5. *Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA*
6. *Division of Hydrologic Sciences, Desert Research Institute, Reno, Nevada 89512, USA*

Although soils are the largest repository of carbon at the Earth's surface, the rates of soil carbon accumulation, transformation and release to the atmosphere and surface waters remain a key uncertainty in forecasts of global change. Within the soil environment, residual plant material is transformed into a continuum of organic products of variable accessibility and reactivity. At the watershed scale, averaging over a variety of these soil reaction networks may obscure critical processes; whereas individual soil profiles provide a limited window into the ensemble of pathways that ultimately determines carbon fluxes to the atmosphere and surface waters. To address how collections of spatially and temporally linked reaction networks are manifest at larger scales and the consequences of scale for process-based models, we are studying C fluxes from the soil profile (0.3 to 2 m²) to the watershed (85 km²) scale (0.005 to 0.1 m²) within the LBNL SFA East River, CO watershed study site.

At the watershed scale, concentration-discharge relationships show considerable hysteresis, with dissolved organic carbon (DOC) fluxes dominated by the seasonal peak in discharge associated with snowmelt. The hysteresis behavior remains remarkably similar for DOC across multiple years. Evaluation of sub-watershed solute dynamics indicates that hillslope aggregation controls solute delivery and increasing discharge is thus flushing DOC that accumulated in the shallow soil during the previous season. Soil profiles generally show decreasing total organic carbon with depth; however, the depth gradients and distributions of organic carbon functional groups vary markedly between different vegetation types (*e.g.*, conifer forest to meadow) and landscape position within one vegetation type (*e.g.*, crest to hillslope). Variability in the carbon distribution with landscape position suggests the importance of soil moisture relative to litter inputs. Soil incubations at variable moisture contents also demonstrate the dependence of CO₂ fluxes on moisture content, with respiration rates increasing with increasing soil moisture from 0 to 66% saturation, followed by a decrease as soils approach saturation. On-going work includes the development of reactive transport descriptions of carbon transformations and how they are mediated by water availability and soil mineralogy.

Collectively, our data suggest that seasonal hydrologic variations create a pulse of DOC to surface waters that temporarily starve the soil environment of labile DOC and provide sub-optimal conditions for heterotrophic respiration, creating a lag time between the hydrologic forcing and the metabolic response. As a result, modeling carbon transformations at the watershed scale will require coupling the temporal dynamics of vertical and lateral water transport with those of soil biogeochemical reaction networks.

The influence of plant and microbial exudates on radionuclide mobility in subsurface environments *University-Led Research under the SBR program*

Brian A. Powell¹ (PI), Kyle Barber¹, Taiwo Biotidara², Timothy A. DeVol¹, Christophe Darnault¹, Musa Danjaji², Rebecca Dozier¹, Nimisha Edayilam¹, Christopher Eley², Kevin Finneran¹, Autumn Gathers², Jazz Geter², Sarah Hennessey¹, Nicole Martinez¹, Fabio Matta³, Dawn Montgomery¹, Stephen Moysey¹, Maryah Nwadeyi², Kindsly Ogujiuba², Nishanth Tharayil¹, Carlie Williams², Ernest M. Wylie¹, Shaniqua Young²,
¹Clemson University, ²University of South Carolina, ³South Carolina State University

This project is part of Department of Energy, Experimental Program to Stimulate Competitive Research (EPSCoR) Implementation Grant “*Radionuclide Waste Disposal: Development of Multi-scale Experimental and Modeling Capabilities*”. The key issues to be addressed include identifying source terms for contaminants in geologic disposal scenarios, determining the chemical speciation of risk-driving radionuclides (*e.g.*, Np, Tc, Cs, U, I) within engineered waste forms and natural subsurface environments, delineating the biogeochemical and physical processes through which contaminant transport is manifested, and predicting contaminant mobility across wide temporal and spatial scales.

This presentation specifically addresses the influence of microbial and plant exudates on radionuclide mobility. The risk driving radionuclides ⁹⁹Tc, ²³⁷Np, ¹³⁷Cs, and ²³⁸U were selected to represent a wide range of geochemical behavior. We have examined the influence of a variety of factors on radionuclide mobility including ionic strength, pH, and the presence of microbial or plant exudates. Comparison of baseline distribution coefficients to distribution coefficients in the presence of ligands such as oxalate, citrate, riboflavin, and catechol showed that high ligand to nuclide concentration ratios produced enhanced mobility, dissolution of native uranium, increased sorption of neptunium and to a lesser extent technetium and minimal effects of cesium behavior. Ionic strength had the greatest influence on Cs partitioning which is consistent with Cs sorption via ion exchange.

Further experiments have examined the influence of plant activity on radionuclide uptake in hydroponic systems. We studied the changes in composition and rate of exudation of metabolites from roots of *Andropogon spp.* exposed to different forms of phosphorous (P) fertilization. Plants were initially grown with available forms of nutrients and were transferred to different nutrient treatments of varying P bioavailability. There were significant and consistent shifts in the metabolic profiles in roots within 36 hours after exposure to various nutrient treatments.

These studies provide insight into the potential effects of plant and microbial exudates on radionuclide mobility and provide necessary data for further miscible displacement experiments and numerical values for modeling efforts which will utilize a unique set of imaging tools to monitor radionuclide transport through soils in 2D and 3D.

Project: Radionuclide Waste Disposal: Development of Multi-scale Experimental and Modeling Capabilities. This material is based upon work supported by the U.S. Department of Energy Office of Science, Office of Basic Energy Sciences and Office of Biological and Environmental Research under Award Number DE-SC-00012530

Understanding Technetium Transport in Porous Media with Batch Geochemical Tests, 4D Emission Imaging Experiments and Modeling Studies

University-Led Research under the SBR program

Rebecca Dozier¹, Kyle Barber¹, Dawn Montgomery¹, Bryan Erdmann¹, Allison Sams¹, Mine Dogan¹, Ruud Ramakers², Harald Groen², Freek Beekman², Brian A. Powell¹, Timothy A. DeVol¹, Stephen Moysey¹, Christophe Darnault¹, Larry Murdoch¹

¹*Clemson University, Environmental Engineering and Earth Sciences*

²*MILabs, Utrecht, The Netherlands*

In this work key parameters controlling technetium (Tc) transport in porous media will be quantified and modeled. Particular focus will be on how transitions in redox state are related to the transport and fate of Tc in the environment. Fundamental geochemical controls have been investigated in equilibrium and kinetic batch sorption studies and have shown substantial differences under oxic versus anoxic conditions as well as in transitions between these conditions. It has also been shown that the amendment of the porous media with strong reducing agents, such as titano-magnetite nanoparticles, can substantially enhance the sorption behavior. This fundamental understanding was then transitioned to column-scale studies intended to investigate the interplay between geochemical conditions and the flow regime. Initial experiments focused on developing and evaluating a novel, one dimensional gamma-ray scanning system to monitor the distribution of Tc-99m within the column over time. While ^{99m}Tc was found to be a useful tracer for one-dimensional transport, we have further investigated the use of SPECT (single-photon emission computed tomography) for 4D (3D with time-lapse) emission imaging of ^{99m}Tc distributions within a column. The value of SPECT imaging, when combined with computed tomography scans of the material, is that it is possible to both image transport behavior in 3D and related this to the structural characteristics of the porous medium, such as preferential flow paths. We are implementing reactive transport models in COMSOL to both improve the design of SPECT imaging experiments as well as to understand how redox transitions affect the local mobility of Tc. One case study, for example, integrates our findings throughout the project by predicting the Tc concentration distributions we might expect in the vicinity of a redox active inclusion (i.e., a zone impregnated with titano-magnetite particles). The model clearly shows a dynamic interplay between the availability of oxygen and Tc reactants, which are controlled by the flow system, and the reactive zone in the column. SPECT imaging experiments are now being designed to validate these modeling results, which are parameterized based on the results of the batch and column experiments.

Project: Radionuclide Waste Disposal: Development of Multi-scale Experimental and Modeling Capabilities. This material is based upon work supported by the U.S. Department of Energy Office of Science, Office of Basic Energy Sciences and Office of Biological and Environmental Research under Award Number DE-SC-00012530

Development of a Self-Consistent Model of Plutonium Sorption: Quantification of Sorption Enthalpy and Ligand-Promoted Dissolution

University-Led Research through SBR program

B.A. Powell (PI), Y. Arai (Co-PI), E. Black, H. Emerson, K. Peruski, R. Pope—*Clemson University*

U. Becker (Co-PI) S. Fernando, S. Park, J. Zhang—*University of Michigan*

D.I. Kaplan (Co-PI), *Savannah River National Laboratory*

The overarching objective of this work is to develop a thermochemical model of Pu sorption to minerals and sediments that incorporates aqueous and solid phase speciation, redox reactions, and the influence of organic ligands. This has been done using a suite of techniques including variable temperature batch sorption, x-ray absorption spectroscopy, quantum mechanical modeling, and isothermal titration calorimetry. In the final year of this project we have utilized the conceptual and quantitative models describing Np and Pu speciation in subsurface environments to describe the mobility of Pu in a series of field lysimeter experiments called the Radiological Field Lysimeter Experiment (RadFLE_x) at the SRS. Analysis of effluent samples from field lysimeters after exposure to 3 years of natural rainfall showed no mobilization of Pu above detection limits. Furthermore, measureable concentrations of Np in the effluent were only found from lysimeters with Np(V) sources. Lysimeters containing Np(IV)O₂ did not have any measurable concentrations of neptunium in the effluent. These findings are supported by laboratory and computational investigations of the strong association of tetravalent actinide species with mineral surfaces. After coring several Pu bearing lysimeters, little transport of Pu had been observed and greater than 99% of the Pu appeared to have remained within the source. There was a greater downward migration of the Pu^VO₂(NH₄)(CO₃)(s) source after just 2 years in the field compared with previously observed transport from Pu(IV) and Pu(III) sources after 11 years in the field. This behavior is consistent with both the enhanced mobility of pentavalent actinides relative to other actinides as well as reduction of Pu(V) to Pu(IV) leading to formation of Pu(IV) surface complexes or Pu(IV) (hydr)oxide precipitates. However, as transport of Pu(V) sources was slightly greater than other oxidation states, it is likely that the slightly enhanced transport observed within the lysimeters is due to transport of Pu as Pu(V) prior to reduction to Pu(IV). In addition, the presence of organic matter decreased the mobility of Pu(V). Although further investigation is needed, this could be due to enhanced reduction of Pu in the presence of organic matter leading to increased sorption to minerals or complexation of Pu with organic matter associated with the bulk minerals. These field lysimeter observations highlight the importance of Pu reduction as a major factor limiting the environmental mobility of Pu in environmental systems.

COLLABORATIVE RESEARCH: NATURAL ORGANIC MATTER AND MICROBIAL CONTROLS ON MOBILIZATION/IMMOBILIZATION OF I AND PU IN SOILS AND WATERS AFFECTED BY RADIONUCLIDE RELEASES IN USA AND JAPAN

Peter H. Santschi¹, Chen Xu¹, Saijin Zhang¹, Kathleen Schwehr¹, Daniel I. Kaplan², Chris M. Yeager³

¹ Laboratory for Environmental and Oceanographic Research, Department of Marine Sciences, Texas A&M University, Galveston, Texas 77551

² Savannah River National Laboratory, Aiken, SC 29808

³ Los Alamos National Laboratory, Los Alamos, NM 87545

¹²⁹I is among the top three risk drivers at DOE Low Level Waste or High Level Waste disposal sites (such as SRS) due to its perceived high environmental mobility, large inventory (high fission yield), high toxicity, and long half-life (16M years). Additionally, it is one of the key radionuclides driving uncertainty with the secondary waste generated from the waste-water treatment facility at the Fukushima Daiichi Nuclear Power Plant (FDNPP). ¹²⁹I exists as iodide, iodate, and organo-iodine. The human and environmental risks associated with Pu disposal, remediation, and nuclear accidents scenarios stems mainly from the very long half-lives of several of its isotopes. The SRS is holding one-third of the nation's Pu inventory. Release of Pu isotopes into the atmosphere and subsequent deposition on the Fukushima Prefecture after FDNPP accident has been reported.

Significant progress has been made over the last 10 years in understanding radioiodine chemistry in groundwater and waste streams as a result of our breakthrough in iodine species detection. This analytical method can detect stable or radioactive iodine at ambient concentrations using standard laboratory equipment. We have shown for the Savannah River Site, Hanford, and Fukushima, that each of the three iodine species has vastly different chemical properties, including their tendency to remain mobile, to adsorb to solids or co-precipitate. Ambient Pu concentrations and isotopic ratios were determined with ICP-MS and alpha spectrometry, in samples collected from both SRS and Fukushima Prefecture.

Sediment Pu concentrations in the SRS F-Area wetland were correlated to total organic carbon and total nitrogen contents and even more strongly to hydroxamate siderophore (HS) concentrations. HS was detected in the particulate or colloidal phases of the sediments but not in the low molecular fractions (< 1000 Da). Water-extractable Pu containing macromolecules were separated via isoelectric focusing (IEF) and assessed via ESI FTICR-MS. Results suggested the presence of HS functionalities in the Pu containing IEF extract. While HS is a very minor component in the sediment, its concentrations greatly exceeds that of ambient Pu. ^{239,240}Pu concentrations in soil samples with different land use types as well as iodine speciation in river water and rainwater northwest of the FDNPP were well correlated to soil organic matter (SOM) content. SOM concentrations and Eh were positively, and pH was negatively correlated to ¹²⁷I concentrations in surface water and rain samples.

Applications of Isotope and Noble Gas Analyses for Water Resources Management

Ate Visser, Lawrence Livermore National Laboratory, visser3@llnl.gov

In the US, 306 billion gallons of fresh water are withdrawn annually from either groundwater or surface water, for domestic use, agriculture, industry or energy production. The relative importance of these sources varies by state, from 80% groundwater reliance in Kansas, to 97% surface water reliance in West Virginia.

Groundwater is a stable, but finite resource. Overdraft threatens groundwater resources if extraction rates exceed recharge. Noble gas and isotopic signatures in groundwater can reveal the recharge mechanisms and conditions. The threats of contamination of groundwater by agricultural land use or point sources can be evaluated from groundwater travel times determined by tritium-helium or other age tracers. A geostatistical analysis of nearly 4000 tritium-helium ages and noble gas concentrations analyzed at LLNL showed that recharge in southern California is dominated by river bank filtration, irrigation return flow, and managed aquifer recharge. Areas of young groundwater coincide with Hydrologically Vulnerable Areas, as independently determined by the State Water Boards.

Although surface water is annually renewed, its availability is seasonally variable and uncertain due to future climate and environmental change. An enhanced understanding of the response and subsurface storage of headwater catchments through water residence-time studies can improve drought-vulnerability assessments. Preliminary results of tritium analyses at the Southern Sierra Critical Zone Observatory show a disconnect between stream water and vegetation uptake in August. Streams discharge decade-old water, while plants transpire recent summer precipitation. “Banking” surface water in subsurface reservoirs provides an economical opportunity to increase the reliability of water supply. The application of water banking has been limited by a lack of knowledge of groundwater/surface-water interactions, recovery efficiency, and water quality concerns. Water recovery efficiency was studied at an Aquifer Storage and Recovery (ASR) well in Woodland (CA) using introduced xenon as a tracer. In this case, 95% of the xenon was recovered after extraction of three injection volumes. Xenon samples were analyzed on a LLNL-developed benchtop Noble Gas Membrane Inlet Mass Spectrometer (NG-MIMS), greatly reducing the cost and turnaround time compared to traditional noble gas mass spectrometry. An introduced xenon tracer experiment at an artificial recharge pond in Fremont (CA) demonstrated the subsurface travel time towards a drinking water production well met the public health criteria. These and other examples demonstrate the benefit of isotope and noble gas tracer studies for water resources research and management.

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Potomac, MD 30854

Systematic Investigation of the Biogeochemical Stability of Iron Oxide-Bound Organic Carbon: Linking Redox Cycles and Carbon Persistence

Yu Yang, University of Nevada, Reno (yuy@unr.edu) (PI); **Eric E. Roden**, University of Wisconsin, Madison (Co-PI); **Daniel Obrist**, Desert Research Institute (Co-PI); **Annie B. Kersting**, Lawrence Livermore National Laboratory (Co-PI); **Baohua Gu**, Oak Ridge National Laboratory (Co-PI)

Our core hypothesis is that the degradation rate of soil organic carbon (OC) during aerobic-anaerobic redox cycles is governed by the amount of iron (Fe)-bound OC, and the ability of microbial communities to utilize OC as an energy source and electron shuttle for Fe reduction that in turn stimulates reductive release of Fe-bound labile dissolved OC. We have been testing our hypothesis systematically using model Fe-OC complexes, natural soils, and microcosm system.

We have initiated studies of the dynamics of Fe and OC in hematite-OC and ferrihydrite-OC complexes during redox reactions. We found that hematite-bound aliphatic C was more resistant to reduction release, although hematite preferred to sorb more aromatic C. Resistance to reductive release represents a new mechanism that aliphatic soil OC was stabilized by association with Fe oxide. To the other side, pyrogenic OC can facilitate the reduction of hematite, by enhancing extracellular electron transport and sorbing Fe(II). For ferrihydrite-OC co-precipitates, the reduction of Fe and release of OC was closely governed by the C/Fe ratio in the system. Based on the XPS, XANES and XAFS analysis, the transformation of Fe speciation was heterogeneous, depending on the conformation and composition of Fe-OC complexes. Fe-bound OC was more thermally resistant compared to free OC, indicating the strong impact of association with Fe on the conformation of OC. Other experiments examining the mobilization and degradation of Fe-bound OC by natural wetland soil microbial communities are underway.

For natural soils, we investigated the quantity, characteristics, and reactivity of Fe-bound OC in soils collected from 14 forests in the United States. Fe-bound OC contributed up to 57.8% of total OC in forest soils. Under the anaerobic reactions, the reduction of Fe was positively correlated to the electron accepting capacity of OC. We also have collected tundra soil from Toolik (Alaska), and started microcosm experiment for studying the response of OC stability and Fe redox reaction to climate change.

Our findings so far highlight the closely coupled dynamics of Fe and OC, with broad implications on the turnover of OC and biogeochemical cycles of Fe. For our next step, we will investigate the transformation of Fe and OC and dynamics of microbial community, when the model Fe-OC complexes and natural soils are exposed to anaerobic-aerobic transitions. Furthermore, the molecular- to microcosm-scale experimental studies will be integrated with model simulations.

UNIVERSITY - TES ABSTRACTS

Dryland feedbacks to future climate: Strong interactions among climate, biota, carbon cycling, and energy balance

Jayne Belnap, Scott Ferrenberg, Colin Tucker, Austin Rutherford, Tom Painter, Sasha Reed

Like all ecosystems, drylands are made up of multiple classes of biota with varied physiologies, survival strategies, and life history traits. A factor that binds dryland organisms together is the harshness of their environment, and that these ecosystems that are characterized by high temperature and aridity are also predicted to become hotter and drier still. Here we present data from a variety of timescales that show how different climate drivers (e.g., increased temperature and multiple altered precipitation treatments) affect the community composition, carbon cycling, and energy balance of a dryland on the Colorado Plateau, USA. Using automated CO₂ flux data from climate manipulation plots, we show substantial exchange of CO₂ between biological soil crusts and the atmosphere. Our recent data highlight how these biocrust CO₂ fluxes are partitioned into net primary productivity and respiration, how these discrete fluxes are differentially affected by increased temperature, and how they are temporally decoupled from the fluxes of vascular plants. This new insight allows us to create dryland biogeochemical models that explicitly include biocrusts, and to test hypotheses about how future climate will affect dryland carbon cycling, both via changes to existing communities and through shifts in community composition. Interestingly, such community shifts not only affect the cycling of carbon and nutrients, but also have strong effects on surface albedo. We have combined our results with global biocrust distribution datasets to estimate radiative forcing effects of predicted climate-induced changes to biocrust communities, and have found incredibly strong negative forcing potential under future climate scenarios. In addition, we have discovered strong patterns between interannual variability in climate and climate manipulation treatments. For example, while the cover, phenology, and physiology of vascular plant species are significantly affected by experimental warming, the interannual variation in climatic extremes has a stronger overall effect on the vegetation community than warming treatments alone. Our results suggest background rates and magnitudes of climate change will interact with extreme climate events to shape future vegetation community structure and ecology. Taken together, these data represent a significant step forward in our understanding of and capacity to forecast how different dryland organisms, biogeochemical cycles, and energy fluxes will respond to a range of future climates.

Modeling the impact of hydraulic redistribution on carbon fluxes and storage using CLM4.5 at four AmeriFlux Sites

TES program (PI Cardon)

Zoe G. Cardon, The Ecosystems Center, Marine Biological Laboratory, Woods Hole, MA 02543, zcardon@mbl.edu

Congsheng Fu, Dept. of Civil and Environmental Engineering, University of Connecticut, Storrs, CT 06269, cof13001@engr.uconn.edu

Guiling Wang, Dept. of Civil and Environmental Engineering, University of Connecticut, Storrs, CT 06269, gwang@engr.uconn.edu

In seasonally-dry ecosystems, when gradients in soil water content develop, plant root systems can serve as conduits for water flow from wet to dry soil (along the water potential gradient). This “hydraulic redistribution” (HR) of water affects landscape hydrology and plant physiology, but is not included in the current generation of standard dynamic global vegetation and earth system models. It has long been hypothesized that HR’s impact on soil moisture profiles also inevitably affects rhizosphere soil microbial activity, and thus heterotrophic soil respiration, carbon cycling, nutrient cycling, and nutrient availability to plants in seasonally-dry systems. Recent field evidence assaying microbial nitrogen cycling activity in dry Utah soils supports this idea. HR thus potentially can affect carbon cycling and land-atmosphere carbon exchange through two pathways: (1) by directly stimulating plant physiology (e.g. enhancing stomatal conductance and thus increasing photosynthesis), and (2) by affecting rhizosphere microbial activity in the soil profile, and therefore the magnitude of heterotrophic soil respiration and/or nutrient cycling rates and nutrient availability to plants. We modified the Community Land Model 4.5 with Century-based soil carbon and nitrogen pool kinetics to include the Ryel et al. 2002’s model of hydraulic redistribution (HR), and we investigated changes in modeled carbon fluxes and storage at four Ameriflux sites where HR is known to occur: US-Wrc (Douglas fir in Washington State), US-SRM (savanna in Arizona), US-SCf (oak-pine forest in Southern California), and BR-Sa1 (evergreen broadleaf tropical forest in Brazil). Model simulations with HR can better capture the net carbon exchange between ecosystem and the atmosphere (NEE) measured at the US-Wrc, US-SRM, and BR-Sa1 sites. The model results indicate that HR tends to increase GPP and enhance plant growth at all four sites, and reduce the temporal fluctuation of soil carbon storage at the three forest sites. The HR-induced increase of GPP is limited by nitrogen, and that limitation is the smallest at the Amazon BR-Sa1 site. HR influences the modeled ecosystem carbon dynamics through: (1) improving plant water availability thus supporting stomatal opening therefore photosynthesis, and (2) through enhanced nutrient availability caused by enhanced soil microbial activity due to HR-induced increase of moisture in shallow soils. CLM4.5 also includes a fire module, and we found that HR also modified fire susceptibility during the dry season. Of these three pathways, water availability affecting plant physiology played the dominant role in modeled effects of HR on carbon cycling.

Molly Cavaleri

Tropical Response to Altered Climate Experiment (TRACE): adventures in warming a wet tropical forest in Puerto Rico

Although tropical forests account for only a fraction of the planet's terrestrial surface, they exchange more carbon dioxide with the atmosphere than any other biome on Earth, and thus play a disproportionate role in the global climate. In the next 20 years, the tropics will experience unprecedented warming. With a Coupled Model Intercomparison Project Phase 5 analysis, we found that model variability in projected net ecosystem production was nearly 3 times greater in the tropics than for any other latitude, thus showing exceedingly high uncertainty in projected tropical responses to this imminent climatic shift. Through a review of the most current literature, we concluded that manipulative warming experiments are vital to accurately predicting future tropical forest carbon balance. Our preliminary data from a wet tropical forest canopy in Puerto Rico shows that photosynthetic optima already exceed maximum leaf temperatures, indicating a decline in carbon assimilation at mid-day temperatures which may be exacerbated by further warming. Yet, it is unknown to what extent tropical species will be able to acclimate, thus mitigating this trend of decreasing the carbon sink behavior of tropical forests. To address these critical research needs, we have initiated the Tropical Response to Altered Climate Experiment (TRACE) in a wet tropical forest in Puerto Rico (El Yunque National Forest). Our primary objectives are: 1) to investigate thermal acclimation potential of mature tropical tree canopy foliage physiology using canopy access towers, branch warming techniques, and chamber gas exchange measurements, and 2) to assess the effects of warming on carbon and nutrient cycling and storage in tropical forest soils with a field warming experiment: the first of its kind in any tropical forest. Here, we present pre-treatment data and report on progress of experimental infrastructure. Results of this research will ultimately represent a significant step forward in our understanding and ability to effectively model tropical forest responses to a warmer world.

Understanding the Response of Photosynthetic Metabolism in Tropical Forests to Seasonal Climate Variations

Dennis G. Dye¹, Scott R. Saleska², Valeriy Ivanov³, Alfredo Huete⁴, Jin Wu², Loren Albert², Rodrigo da Silva⁵, Bruce Nelson⁶, Luiz Aragao⁷, Marciel J. Ferreira⁸

¹U.S. Geological Survey, Western Geographic Science Center, ²University of Arizona, Dept. of Ecology and Evolutionary Biology, ³University of Michigan, Dept. of Civil and Environmental Engineering, ⁴University of Technology, Sydney, Australia, ⁵Federal University of West-Para (UFOPA), Santarem, Brazil, ⁶National Institute of Amazonian Research (INPA), Brazil, ⁷National Institute for Space Research (INPE), Brazil, ⁸Federal University of Amazonas (UFAM), Brazil

This U.S.-Brazil collaboration investigates a fundamental question in Earth system science and tropical forest ecology: what controls the response of photosynthesis in evergreen tropical forests to seasonal variations in climate? This question reflects a scientific problem that heretofore could not be solved with confidence. The seasonal patterns of photosynthesis in Amazon tropical forests simulated by state-of-the-art Earth system models disagree with observations: satellite-based records of forest “greenness” and tower-based measurements of carbon dioxide exchange. Models assume that lower precipitation in tropical forests means less plant-available water and less photosynthesis, yet the observations show that production remains constant or increases in the dry season. Such disagreement highlights a major source of uncertainty in efforts to understand global carbon-climate interactions and to forecast future climate: current Earth system models do not adequately account for the extent, magnitude, and controls on photosynthetic seasonality in evergreen tropical forests. Our research solves this problem by providing new knowledge and deeper understanding of seasonal climate-photosynthesis relations in tropical forests of the Brazilian Amazon, across a gradient of dry season length between Manaus (with a short dry season) and Santarem (with a long dry season). The methods involve intensive field campaigns to measure physiological and ecohydrologic properties of leaves and trees, camera systems to monitor forest growth at tree crown and canopy scales, and photosynthesis modeling that accounts for the 3-dimensional forest structure and light environment. Here we present recent, significant findings from the research.

Analysis of hydraulic relations in trees at our Amazon study sites, using ecohydrologic data (stem sapflow, water potential, and gas exchange), reveal distinct hydraulic strategies that convey different levels of resilience to short- (diurnal) and longer-term (seasonal) water stress periods. These hydraulic strategies appear to be inter-related with tree growth and non-structural carbohydrate dynamics, contributing to the understanding of trait coordination at the whole-plant scale. The integrated individual responses over a range of wood density and light exposure conditions show temporal changes of the forest response to 2015-2016 El Nino conditions. Our tower-based cameras enabled investigation of the phenology (seasonal pattern) of leaf dynamics in tree crowns and their relation to patterns of carbon dioxide flux. The analysis showed the synchronization of new leaf growth with dry season litterfall shifts canopy leaf composition toward younger, more light-use efficient leaves, thus explaining large seasonal increases (~27%) in ecosystem photosynthesis. Accounting for age-dependent variation among individual leaves and crowns is therefore necessary for reliable modeling of the seasonal dynamics of photosynthesis in the entire ecosystem. These results highlight the importance of tree hydraulic strategies and leaf level phenology in regulating land surface fluxes of carbon and water, and associated feedbacks to climate. This new knowledge and understanding can guide improvements in the treatment of tropical forest systems in models of the global carbon cycle and the Earth’s climate system.

Topographic Controls on Soil Respiration and Fine Root Distribution at the Shale Hills Critical Zone Observatory

Alexandra Orr, Thomas Adams, Jason Kaye and David Eissenstat

In the following abstract, Thomas Adams assisted myself, Alexandra Orr, in the collection of the all of the data analyzed. Additionally, Jason Kaye and David Eissenstat provided guidance in the research design, analytical methods, data analysis, and presentation materials.

Fluctuations in soil moisture caused by climate change could profoundly impact belowground carbon dynamics. However, most studies investigating the impact of soil moisture fluctuations on belowground carbon processes are plot-level experiments, with minimal topographic variation. Scaling these experiments to the landscape level is challenging because complex topographic variation drives spatial and temporal patterns of soil water content. We examined how variation in soil moisture along with other factors such as temperature, soil thickness and aboveground net primary production, influenced root distribution and soil respiration across a first-order catchment of diverse topography (Shale Hills CZO).

During the 2014 field season, 250 soil cores were taken to a maximum depth of 165cm. Soil cores were divided into depth increments of 20 to 40 cm, homogenized then split so that each half contained roughly equal soil and root constituents. One half of the sample was analyzed for root distribution, and the other half was analyzed for soil properties. Root samples were separated into absorptive roots (1st to 3rd order roots) and transport roots (>3rd order roots) and then length and average diameter determined. Soil samples were analyzed for NO₃⁻, NH₄⁺, soil organic matter, rock content, exchangeable acidity, C:N and CEC. Other measures including LAI, leaf litter mass and tree diameter were also determined within each plot to compare aboveground patterns with root distribution. Initial results show complex variations in root distribution that may be most influenced by the interaction of rock and water content in the soil.

During the 2015 field season, weekly measurements of soil respiration, water content and temperature (both at a 5cm depth) were taken at 200 locations throughout the catchment. Within a transect across a hill slope, an additional eight respiration chambers recorded measurements every 15 minutes. Initial results show that hillslope swales exhibited higher seasonal respiration rates than the planar slopes, ridge tops and valley floor. Soil moisture tended to be highest in the valley but did not differ between other slope positions. Soil moisture limited soil respiration at levels of saturation but enhanced soil respiration during rewetting events.

Collectively, these preliminary results suggest that there is high spatial and temporal variation in root length density and soil respiration that are not easily predicted by simple metrics such as slope position or soil moisture.

Title: Spatial Variation in Microbial Processes Controlling Carbon Mineralization within Soils and Sediments

Scott Fendorf (PI), Stanford University
Marco Keiluweit, Stanford University
Michael Schaefer, Stanford University
Chris Francis, Stanford University
Markus Kleber, Oregon State University
Thomas Wanzek, Oregon State University
Peter Nico, Lawrence Berkeley National Laboratory

Approximately 3300 Pg of carbon (C) are stored in soils as organic matter, which is three-times the amount stored in the atmosphere. An important control on soil organic matter (SOM) storage is the mineralization (oxidation) rate, which is affected by climatic factors (particularly temperature and rainfall) influencing microbial metabolic rates as well as SOM chemistry, mineral-organic associations, and physical protection. What remains elusive is to what extent constraints on microbial metabolisms induced by the respiratory pathway, and specifically the electron acceptor in respiration, control overall rates of carbon mineralization in soils. The complex physical structure of soils and sediments results in an abundance of redox environments even within seemingly aerobic systems. Therefore, factors limiting oxygen diffusion and availability such as soil texture and aggregate size (soil structure) may be central controls on microbial C mineralization rates.

Combining micro-scale laboratory experiments with field-scale observations, we find that texture-induced oxygen diffusion limitations create anaerobic microsites within seemingly well-aerated soils, shifting microbial metabolism to less efficient anaerobic SOC oxidation pathways.

In both saturated and unsaturated systems, microsensor measurements in combination with gas flux measurements showed that particle size exerts a strong control on the extent of the anaerobic volume, thereby causing an overall decrease in OM oxidation rates. In model aggregates, we determined the distribution of operative microbial metabolisms and their cumulative impact on SOM transformations and overall oxidation rates within anaerobic microsites. Metabolic profiling showed that texture-induced anaerobic microsites reduced SOC oxidation rates by an order of magnitude relative to aerobic rates, with Fe reduction contributing more than 75% of the overall metabolism. Density separations in combination with C 1s NEXAFS spectroscopy and high-resolution FT-ICR-MS showed that texture-induced anaerobic microsites resulted in the preferential preservation of reduced (electron-rich) organic carbon compounds (both dissolved and particulate), a result corroborated by field measurements across multiple sites.

Collectively, our results suggest that anaerobic microsites are an underappreciated OM protection mechanism in upland soils. Removing anaerobic metabolic constraints through increased soil aeration (e.g., through changes in precipitation patterns or land use) will stimulate microbial oxidation of this inherently bioavailable SOC pool. Models that attribute the effects of texture merely to ‘mineral protection’ may therefore underestimate the vulnerability of soil C to global change impacts.

High latitude peatlands contain nearly half of Earth's soil carbon pool and represent a particularly significant terrestrial carbon sink. As result of their anoxic conditions, peatlands are simultaneously a large C sink but also a major source of CH₄ to the atmosphere. The greatest rates of warming are occurring at high latitudes and warming is predicted to accelerate the loss of the C stored in peat as a result of faster rates of decomposition. The magnitude of forms of these C losses as CO₂ and CH₄ remains highly uncertain.

To address these uncertainties we have proposed a measurement and modeling activity for the DOE-funded *Spruce and Peatland Response Under Climatic and Environmental Change* (SPRUCE) experiment in the Marcell Experimental Forest, MN. The field-based measurement activity will test four empirical hypotheses (EH) relating CO₂ and CH₄ emissions to experimental warming (0 to +9 °C in 2.25 °C increments) and elevated CO₂ (~850ppm):

EH1: Biogenic emissions of CO₂ and CH₄ will increase significantly at eCO₂ compared to aCO₂.

EH2: The rate of acetoclastic methanogenesis relative to hydrogenotrophic methanogenesis will increase across the gradient in warming.

EH3: Reductions in water table height increase the depth of the aerobic layer thereby decreasing the rate of net methanogenesis and the CO₂-to-CH₄ ratio of emissions from the peat surface.

EH4: Elevated CO₂ significantly increases autotrophic and heterotrophic respiration in proportion to the level of experimental warming and compared to that observed at ambient CO₂.

The modeling activity will relate the field measurements to two modeling hypotheses that are relevant to identifying essential attributes of next generation ecosystem and earth system models: (1) models need explicit representation of agents (microbes and/or enzymes), environment (e.g., temperature and moisture), and substrate supply (including substrate diffusion) to skillfully simulate decomposition and heterotrophic respiration at any spatial or temporal scale; (2) because O₂ diffusion and consumption in soil drive aerobic and anaerobic microbial respiration, it should be possible to simulate both CO₂ and CH₄ fluxes simultaneously using the same soil physics model structure and carbon availability. The proposed data-model integration can also identify the types of observations needed to improve model parameterization, thus coupling *modeling* with observational and experimental measurements (i.e., *ModEx*). This poster will present initial field results and the formulation of our modeling platform.

Regional groundwater systems convey deep crustal carbon into rainforest water, air, and plants in Costa Rica

David P. Genereux¹, Steven F. Oberbauer², Christopher L. Osburn¹, Diego Dierick², Diana Oviedo Vargas¹

1: Marine, Earth, and Atmospheric Sciences, NC State University

2: Biological Sciences, Florida International University

This project focuses on the discharge of high-carbon regional groundwater into streams and wetlands in a Costa Rican rainforest, and resultant impacts on ecosystem carbon pools and fluxes. Streams, springs, and swamps that receive inputs of old, high-DIC regional groundwater function as hot-spots of C flux in the lowland rainforest landscape. The importance of this hot-spot C transfer driven by regional groundwater has been demonstrated by comparing C concentrations, fluxes, chemistry, and isotopes in two adjacent rainforest watersheds at La Selva Biological Station: the Arboleda and Taconazo. Both watersheds have young low-DIC local groundwater, but the lower Arboleda also receives inputs of old high-DIC regional groundwater.

Old high-DIC regional groundwater:

- is responsible for an average DIC flux into the Arboleda watershed "from below" of $\sim 820 \text{ g C m}^{-2} \text{ yr}^{-1}$, a value 22–30% of the magnitude of whole ecosystem respiration at La Selva
- increases stream export of total DIC by 70x
- increases stream water CO_2 concentration by 4-6x in the dry season and 5-11x in the wet season (average increase is 7x)
- increases CO_2 degassing flux by 7-15x in the dry season and 4-8x in the wet season (average increase is 8.5x)
- has no significant effect on stream methane concentration or degassing flux (regional groundwater at La Selva is oxic despite a long subsurface residence time of ~ 3000 yr)
- lowers the stream DOC concentration slightly (old regional groundwater is lower in DOC than young groundwater) but increases DOC export by a factor of 3.5 (because of the large additional water throughput)
- causes differences in stream water DOM chemistry (e.g., leads to less aromatic DOM) at baseflow but not during storm flow.

In the Taconazo, where respiration is the only ecosystem source for CO_2 , $\delta^{13}\text{C}-\text{CO}_2$ vs. $1/[\text{CO}_2]$ give a typical straight-line Keeling plot defined by atmospheric CO_2 and CO_2 from ecosystem respiration. However, data from the lower Arboleda plot to the upper left of this line toward higher $\delta^{13}\text{C}$ values at higher CO_2 concentration, indicating the contribution of CO_2 from regional groundwater. Also, average $^{14}\text{C}-\text{CO}_2$ in air (n=3) was very low (61% modern) near a stream zone of high gas exchange (weir) in the Arboleda but not in the Taconazo (100%); near the Arboleda stream but far upstream away from the weir, the average was 97%, reflecting a small but non-zero influence of deep crustal C delivered to the Arboleda stream by regional groundwater flow and outgassed there by normal gas exchange processes.

^{14}C data from live understory plant leaves unambiguously show the presence of deep crustal C in modern plants: mean % modern C (n=6) was only 64% for leaves growing near the Arboleda weir, but 102% for leaves growing near the Taconazo weir.

Carbon Dynamics of the Greater Everglades Watershed and Implications of Climate Change

C. Ross Hinkle (University of Central Florida, rhinkle@ucf.edu)

Brian Benscoter (Florida Atlantic University, bbenscot@fau.edu)

Xavier Comas (Florida Atlantic University, xcomas@fau.edu)

DOE-SC0008310

Low-latitude wetland watersheds are a significant component of the terrestrial carbon (C) cycle, but are highly vulnerable to the dual pressures of land use and climate change. We are using the Greater Everglades to evaluate the response of these watersheds to environmental change. Eddy covariance (EC) measurements of CO₂, CH₄, and H₂O were collected along a hydrologic gradient at three sites: pine flatwoods (no CH₄), seasonal depression marsh, and sawgrass peatland. Over the past three years, the flatwoods averaged an uptake of 96 g C-CO₂ m⁻² yr⁻¹ and showed little seasonality. Both wetlands had seasonal patterns related to water depth, with C-CO₂ uptake averaging 131 g m⁻² yr⁻¹ in the depression marsh and 177 g m⁻² yr⁻¹ in the peatland. Methane emissions from the depression marsh (66 g C m⁻² yr⁻¹) were nearly double that of the peatland (38 g C m⁻² yr⁻¹), possibly due to the marsh's more variable water table and shallower organic soils. Evapotranspiration (ET) was also greater in the wetland sites and strongly associated with open water, as canopy biomass reduced water loss from the sawgrass peatland compared to the more sparsely vegetated depression marsh. Leaf gas exchange comparisons suggest potential feedbacks to autogenic wetland drying resulting from shrub encroachment. Shrubs had lower water use efficiency but double the LAI of sedge communities, resulting in net wetland water loss. Closed chambers with OTCs showed increased C exchange with 2-3°C daytime warming, with a 50-60% increase in net C uptake at the depression marsh and flatwoods despite increased ecosystem respiration.

A combination of GPR, gas traps and time-lapse cameras in the field and laboratory are investigating gas build-up and release at high spatial (i.e. centimeter) and temporal (i.e. sub-hourly) scales, as well as how peat thickness and seasonality may influence gas releases. A novel algorithm using ground penetrating radar (GPR) soil surveys and wetland surface area from aerial images estimated depression marsh soils contribute 89 Gg C within the Disney Wilderness Preserve alone. Litter incubations showed surface decomposition was nearly 3x greater in the pine flatwoods (324 g biomass m⁻² yr⁻¹) compared to the wetlands. Root productivity was also greatest in the flatwoods (90 g biomass m⁻² yr⁻¹) compared to the wetlands (10-16 g m⁻² yr⁻¹), with the majority of new roots produced at depths of 4-12 cm. Our findings are informing terrestrial ecosystem models to evaluate the atmospheric forcing of wetland watersheds under future climate scenarios.

Microbial Response to Deep Peat Heating

Kirsten S. Hofmockel, Sheryl Bell, Montana Smith, Allison Thompson, Lisa Bramer, Erik A. Hobbie

Boreal peatlands cover 3% of the earth's surface and contain 1/3rd of the planet's terrestrial carbon stores. As temperatures rise, northern bogs are expected to release more carbon, fueling greater warming. To examine the role of microbial decomposition in the surface of boreal bogs, we monitored extracellular enzyme activity at the Spruce and Peatland Responses Under Climatic and Environmental Change (SPRUCE) experiment in the USFS Marcell Experimental Forest. Carbon-, nitrogen- and phosphorus-degrading extracellular enzymes were measured in a peat heating experiment, where peat at 2 m was warmed as much as 9 °C above ambient temperatures. Two replicate plots were sampled for each heating treatment. Samples were collected when warming began in June 2014 and again in September after 100 days of warming. Potential activity of nine extracellular enzymes was quantified at 0-10, 10-20, and 20-30 cm below the peat surface for each sampling date.

Greatest enzyme activity was in phosphorus > carbon > nitrogen-acquiring enzymes (acid phosphatase > beta-glucosidase > N-acetylglucosaminidase). Generally enzymatic potential was higher in the surface (0-10 cm) and decreased with depth (and increasing moisture). When assessed *in situ*, nitrogen-acquiring enzymes of microbial populations were more sensitive to deep peat heating than carbon- or phosphorus-liberating enzymes. Aminopeptidases were sensitive to warming at 10-20 cm below the peat surface in plots warmed +4.5 °C at depth. Median enzymatic potential for leucine aminopeptidase was 11 times greater in warmed plots than in ambient plots. Similarly, median alanine aminopeptidase potential 10-20 cm below the surface was 4 times greater in warmed plots than in controls. Peptidases contribute to both carbon and nitrogen cycling. Peptidases depolymerize proteinaceous material to liberate amino acids, which can be directly assimilated by both plants and microbes. Peptidases have been identified as the main enzymes involved in short-circuiting the N mineralization pathway, thus supporting the rapid cycling of organic N, particularly in N-limited ecosystems. Our results suggest that peptidases may be particularly sensitive to ecosystem shifts in temperature. Therefore, increased peptidase activity with warming could alter N availability, and in turn alter plant and microbial productivity. Increased organic N cycling in response to warming may be harbingers for longer-term plant community responses and the ecosystem C budget, which will be assessed with future sampling of the SPRUCE experiment.

Atmospheric signatures of large-scale variations in the isotopic fractionation of terrestrial photosynthesis.

Ralph Keeling, Alane Bollenbacher, Steve Piper, Sara Afshar, Scripps Institution of Oceanography

Heather Graven, Imperial College, London

The CO₂ flask program at the Scripps Institution of Oceanography has resolved trends in the ¹³C/¹²C isotopic composition of atmospheric CO₂ from 1977 to present. A major feature of these data is a secular trend towards lower δ¹³C values, known as the carbon-13 Suess effect. The ¹³C Suess effect, like that for ¹⁴C, is driven primarily by the input of CO₂ from fossil fuels. Fossil-fuels are slightly depleted in ¹³C because they were ultimately formed from photosynthesis, which involves selective uptake of ¹²CO₂ over ¹³CO₂. The emission of fossil-fuel CO₂ therefore lowers the atmospheric ¹³C/¹²C ratio. A second important influence on the ¹³C Suess effect is natural back-and-forth exchanges of CO₂ with land and ocean carbon reservoirs. These gross exchanges, also known as "isofluxes" or "disequilibrium fluxes", scramble carbon atoms between reservoirs, thereby spreading the Suess effect into the land and oceans while reducing the atmospheric signal. A third influence is net gains or loss of carbon by the land biosphere, which is depleted in ¹³C because of photosynthesis, similar to fossil-fuels. A sink for excess CO₂ on land therefore offsets the influence of fossil-fuel burning, not just on CO₂ amount, but also on its isotopic composition. In contrast, ocean uptake of excess CO₂ has little influence on δ¹³C of atmospheric CO₂.

Here we update these records and compare them to results of a simple global carbon cycle model which treats the atmosphere and land biospheres as well-mixed reservoirs and the ocean as a 1-D diffusive system. Rather than focusing on using the δ¹³C and CO₂ concentration data to resolve global land and ocean carbon sinks, we instead use the data/model comparison to show that there must exist an additional process, previously neglected, that reduces the atmospheric δ¹³C Suess effect. The need for this process has become more evident as the records have grown in length. We suggest that the missing process is a systematic global increase in the isotopic discrimination of land photosynthesis. This increase has implications for global trends in leaf-level water-use efficiency, which will be discussed.

Title: Functional Aerobic-Anaerobic Metabolic Heterogeneity within Soils

Thomas Wanzek, Oregon State University
Markus Kleber, Oregon State University
Marco Keiluweit, University of Massachusetts—Amherst
Peter Nico, Lawrence Berkeley National Laboratory
Scott Fendorf (PI), Stanford University

Carbon cycling models do not account for organic matter decomposition under conditions where O_2 is limiting. However, the complex physical structure of soils can result in an abundance of anaerobic microsites and associated metabolic gradients even within seemingly aerobic, well-drained soils. If decomposition processes based on alternative electron acceptors are included in carbon cycling models, information is required about 1) the functional extent of soil microenvironments, and 2) how microenvironments are modified by temporal variations in environmental drivers.

Unfortunately the abundance and distribution of metabolically different soil microenvironments is poorly defined. Our approach to resolve this issue is based on the insight that metabolic activity is a progressive consumption of electron acceptors, a feature that can be observed using platinum redox probes. If a suitable number of replicate probes are installed within a soil horizon, then the observed variability is a numerical indicator of microenvironment diversity.

We use the following premises to evaluate and scale outcomes of soil redox metabolic heterogeneity: (1) If structure is the main control on microenvironment heterogeneity, and structure remains constant over time, the variability in redox potentials should be constant. (2) Particle-size distribution and (3) pore network structure are robust predictors of redox variability and thus of the extent to which soil is organized into microenvironments. With these assumption, we characterized the spatial variability of redox potentials by deploying sets of platinum redox probes within standardized soil volumes both in the laboratory and in the field. Redox potentials in both settings were collected over time to capture the effects of seasonal variations in soil temperature and moisture content. Soil structure was parameterized using X-ray computed tomography. We find that metabolic heterogeneity within a soil horizon is minimal when the system is either completely saturated or completely dry (low moisture potentials). High amplitudes of heterogeneity were observed when the system was in transition between those states. Soil pore network structure mainly determines the rates of change and the absolute magnitude, but not the incidence, of redox heterogeneity.

Our data support the hypothesis that episodes of oxygen deprivation may be encountered in “upland” soils. Soil structure data may be useful to constrain the absolute magnitude of anaerobic events, while climatic parameters may serve to predict frequency and duration.

Warming effects on peat column CH₄ dynamics in a Minnesota bog

Jason K. Keller¹, Anya Hopple², Cassandra A. Medvedeff¹, Laurel Pfeifer-Meister², and Scott D. Bridgham²

¹Schmid College of Science and Technology, Chapman University

²Institute of Ecology and Evolution, University of Oregon

TES Program (DE-SC0008092; DE-SC0014416), PIs J.K. Keller (jkeller@chapman.edu) and S. D. Bridgham (bridgham@uoregon.edu)

Northern peatlands store roughly one-third of terrestrial soil carbon and are responsible for a significant fraction of the flux of the potent greenhouse gas methane (CH₄) to the atmosphere. An important question in global biogeochemistry remains whether peatland soil carbon will be released to the atmosphere as CH₄ in response to global change. An answer to this requires a mechanistic understanding of both CH₄ production and CH₄ oxidation. The Spruce and Peatland Responses Under Climatic and Environmental Change (SPRUCE) project will ultimately manipulate temperature (+0, +2.25, +4.5, +6.75 and +9 °C) and atmospheric CO₂ concentrations (Ambient, +850 ppmv) within a northern Minnesota bog. Deep peat heating was initiated in June of 2014; whole ecosystem warming, including above-ground warming, was initiated in August of 2015; and elevated CO₂ treatments will begin in the summer of 2016. This project provides a unique opportunity to investigate the mechanistic controls of both CH₄ production and oxidation.

To explore the controls of CH₄ production, we collected soil cores through the 2 m soil profile in September of 2014 and June of 2014 (during deep peat heating) and in August and September of 2015 (during whole ecosystem warming). Soils were incubated anaerobically at in situ temperatures with the addition of a ¹⁴HCO₃⁻ tracer to explore the effects of warming on total CH₄ production as well as hydrogenotrophic and acetoclastic methanogenesis. Warming stimulated net CH₄ production in surface depths, but did not have an effect in deeper soils. However, warming decreased CO₂:CH₄ ratios throughout the peat column, with greatest effects in surface peat. Warming had little impact on the concentrations of fermentation products, including the methanogenic substrates acetate and H₂. Overall, the lack of temperature effects suggest that deep peat soils are resistant, at least initially, to warming.

The same soil cores described above were incubated with ¹⁴CH₄, and preliminary evidence suggests that anaerobic CH₄ oxidation may be occurring in these soils (calculated as the production of ¹⁴CO₂ in these samples). Additionally, the use of an in situ isotope dilution protocol shows promise for measuring net CH₄ oxidation at the ecosystem scale. Taken together, measurements of CH₄ production and CH₄ oxidation in the SPRUCE project will provide important insights into the mechanistic controls of CH₄ cycling in the context of ongoing global change.

The response of belowground carbon turnover and heterotrophic microbial communities to warming in peatlands at the ecosystem scale.

DE-SC0012088, TES Program; Email address: joel.kostka@biology.gatech.edu

Joel E. Kostka¹, Max Kolton¹, Rachel Wilson², Jeff P. Chanton², William T. Cooper², and Chris W. Schadt³, Karis MacFarlane⁴, Tom Guilderson⁴.

¹Georgia Institute of Technology; ²Florida State University; ³Oak Ridge National Lab;

⁴Lawrence Livermore National Lab

High latitude peatlands store approximately 1/3 of all soil carbon(C), but wetland-specific processes are underrepresented in global climate models. Using advanced analytical chemistry, ¹⁴C and ¹³C tracing, and next generation gene sequencing, this project quantifies the response of soil organic matter (SOM) storage, reactivity, and decomposition, and the functional diversity of microorganisms to climate change manipulation in peatlands. The project is being conducted at the Marcell Experimental Forest(MEF), northern Minnesota, where the Oak Ridge National Lab (ORNL) has established an experimental site known as Spruce and Peatland Response Under Climatic and Environmental Change (SPRUCE). In collaboration with SPRUCE investigators at ORNL, new insights will be incorporated into the land component of the Community Earth System Model to improve climate projections.

From June 2014 to June 2015, an experiment known as Deep Peat Heating (DPH) was conducted at SPRUCE whereby soil heating alone was initiated to >2 m depth. Our group evaluated the response of the belowground C cycle and microbial communities in 5 soil warming treatments(+0°C; +2.25°C; +4.5°C; +6.75°C; +9°C). To verify the role of surficial processes in the field CH₄ flux response, we compared the natural abundance $\Delta^{14}\text{C}$ of the porewater dissolved organic carbon (DOC), CO₂ (DIC), and CH₄ with the solid peat. In all plots and depths, the $\Delta^{14}\text{C}$ of CH₄ and DIC were relatively young, ¹⁴C-enriched relative to the peat, and indistinguishable from the $\Delta^{14}\text{C}$ of the DOC. This is consistent with respiration fueled by recent primary production rather than degradation of older catotelm C. The young age and lack of a temperature effect on DOC concentrations belie significant leaching of catotelm C into the dissolved pool after 13 months of warming. The concentration and stable C isotope composition of respiration products (DIC and CH₄) across all temperature treatments were stable within observed environmental variability, supporting the conclusion that warming did not increase deep peat C mineralization. Findings from radiocarbon chemistry are corroborated by parallel analysis of the in situ microbial communities. While microbial community structure and abundance were stable across all temperature treatments, strong vertical stratification was observed in parallel with geochemical evidence of peat decomposition state, corroborating our baseline data published from S1 bog. The potential activity of extracellular oxidative enzymes (phenol oxidases and peroxidases) was also consistent across temperature treatments and years. Our initial results indicate that the large store of deep catotelm C will be resistant to anaerobic degradation under future climatic warming.

Project title: Collaborative Research on Ecophysiological Controls on Amazonian Precipitation Seasonality and Variability

Jung-Eun Lee (Brown University), Joseph Berry (Carnegie Institution for Science), Pierre Gentine (Columbia University), Benjamin Lintner (Rutgers University)

The principal objective of our project is to address how vegetation influences climate variability and precipitation over Amazonian rainforests, with an emphasis on plant physiological controls on deep convection triggering along a geographical water stress gradient. Using a new tool of sun-induced chlorophyll fluorescence (SIF), our study integrates plant physiological observations and climate modeling and aims to decrease the gap between field ecology and climate modeling. This year, we have installed sensors at Manaus site (K34; July-August 2015) and at Rebio Jaru (Ji-Paraná, Rondonia; September 2015).

To investigate the role of water stress on the onset of the rainy season, we have developed high-resolution cloud resolving model (CRM) simulations using a new strategy coupling convective and large-scales. The first results show that the presence of early morning fog reduces the wet season transpiration and carbon uptake over the everwet regions of Amazonia (Anber et al., in press; the top feature story on the DOE Atmospheric Science Research Program's home page right now—Fog and Rain in the Amazon). We have incorporated SIF into CLM (Lee et al., 2015) to constrain energy, carbon and water flux of tropical forests. Additionally, we have been meeting online every other week to fill the knowledge gaps among our interdisciplinary team members, to educate our students and postdocs, and to exchange ideas. Our efforts in the coming year will focus on analyzing data from the field activities and on modeling the interactions of convection and plant physiological processes.

Scaling Biospheric CO₂ Fluxes in the Western U.S. From Site to Region Using the Community Land Model

Henrique F. Duarte¹, John C. Lin¹, Derek V. Mallia¹, Dien Wu¹, Britton B. Stephens², Brett M. Raczka³, Daniel M. Ricciuto⁴, Charles D. Koven⁵, Peter E. Thornton⁴, David R. Bowling³, James R. Ehleringer³

¹University of Utah, Department of Atmospheric Sciences, Salt Lake City, UT

²National Center for Atmospheric Research, Boulder, CO

³University of Utah, Department of Biology, Salt Lake City, UT

⁴Oak Ridge National Laboratory, Oak Ridge, TN

⁵Lawrence Berkeley National Laboratory, Berkeley, CA

Forests in mountainous terrain represent a major carbon sink in the Western U.S. These forests are particularly vulnerable to climate change, which is expected to increase the frequency and severity of droughts, wildfires, and insect damage. Such disturbance events could weaken these forests' capacity to sequester carbon or switch them from a net carbon sink to a source. Despite the relevance of these mountain ecosystems, direct carbon flux measurements with eddy covariance towers are sparse, especially due to difficulties associated with complex topography. Land-surface models, constrained by observed atmospheric CO₂ concentrations, emerge as an alternative for quantifying current carbon fluxes and projecting carbon dynamics into the future.

We carried out simulations with the Community Land Model, Version 4.5 (CLM). The model successfully simulated photosynthetic carbon isotope discrimination and surface-atmosphere exchange of CO₂, water, and heat at two AmeriFlux sites in coniferous forests in the Western U.S.: 1) Wind River (Pacific Northwest) and 2) Niwot Ridge (Colorado). In accomplishing this successful comparison against observations we calibrated key parameters controlling plant-physiology and soil processes within CLM.

Here we expand our CLM simulations to the Western U.S. region, using the same successful strategy we implemented for the site-level runs regarding model spin-up and transient simulations, which account for pre-industrial to present-day changes in atmospheric CO₂ and ¹³CO₂, nitrogen and aerosol deposition, and land-cover change. In order to evaluate CLM performance we used a time-reversed Lagrangian transport model (Stochastic Time-Inverted Lagrangian Transport Model; "STILT") to link CLM carbon fluxes to atmospheric CO₂ concentrations at 3 in-situ CO₂ observations sites in the Regional Atmospheric Continuous CO₂ Network in the Rocky Mountains (Rocky RACCOON). Meteorological fields from a high-resolution Weather Research and Forecasting (WRF) simulation were used to drive CLM and STILT during the summer of 2012, a period characterized by a severe drought in the Western U.S.

We are currently working on the regional calibration of key plant-physiology parameters in CLM, aiming to minimize the differences between modeled and observed atmospheric CO₂ concentrations at the Rocky RACCOON sites. We present results of this initial calibration effort.

Increasing drought-induced forest mortality has been recognized as a global phenomenon. In the Southwestern US, increased temperatures and decreased precipitation have increased drought severity, exacerbated ecosystem stress, and ultimately triggered widespread forest mortality, which is expected to increase dramatically in the coming decades. Such abrupt change can be irreversible when an ecosystem passes a 'tipping point', eliciting a strong non-linear response. Forests and woodlands may be particularly prone to non-linear responses because of strong coupling between hydrological and carbon cycles.

In 2009, we girdled all adult piñon trees on a heavily instrumented 4 ha plot to produce rapid mortality, and have continuously monitored biogeochemical responses there and at a corresponding control site since 2009 to quantify both the consequences of large scale mortality for ecosystem function and rates of recovery. In 2013, our intact control site experienced large scale bark beetle driven mortality, which continued through 2015, giving us the opportunity to compare consequences of natural vs. induced large scale mortality events in this biome. Previous studies suggest that abrupt tree death should "release" soil water ("moisture release hypothesis") facilitating water uptake by surviving woody plants, understory herbs and tree recruits. We report here on new methods we have used to quantify the extent of mortality in PJ woodlands, using high-resolution repeat measurements of vegetation using structure-from-motion (SfM) techniques, and on the ecohydrological results that have emerged from both the natural mortality event and our ecosystem-scale manipulation that test this hypothesis.

Contrary to our expectation that piñon mortality would increase water availability for the remaining trees, total 0-30 cm integrated soil water content under dead piñon and the remaining juniper trees progressively decreased at the girdled site, relative to the control site, from 2010 to 2012, while 0-30 cm soil water under bare, inter-canopy areas between the girdled and control site did not change. As a result of this decrease in soil moisture, sap flow of the remaining trees and total canopy transpiration progressively decreased (juniper sap flow declined faster and more consistently than the remaining small piñon) at the girdled site, relative to the intact control site over this time period.

These results suggest piñon mortality has made this PJ woodland progressively drier and hotter relative to a nearby intact PJ woodland. We propose this could be a result of tree density and site hydrology being linked by unrecognized positive feedbacks, such that the loss of trees can trigger aridification. Such links provides a framework to propose several mechanisms that might explain how piñon mortality could alter the temporal dynamics and spatial distribution of soil moisture to the detriment of surviving plants, and the future trajectory in the structure and function of PJ woodlands. We describe recently funded work will build upon these findings and begin to investigate these mechanisms.

Shrinking stems of marsh plant under elevated carbon dioxide

Meng Lu¹, Bert G. Drake¹, J. Adam Langley^{1,2}, & J. Patrick Megonigal¹

¹Smithsonian Environmental Research Center, 647 Contees Wharf Road, Edgewater, MD 21037, USA

²Department of Biology, Villanova University, 800 E. Lancaster Avenue, Villanova, PA 19085, USA

Abstract: Coastal wetlands are considered as one of the most valuable ecosystems on Earth, yet sea level rise, acidification, pollution and climate change are threatening these fragile systems. Atmospheric carbon dioxide (CO₂) concentration has evidently increased 43% since 1850 and is projected to reach 985 ± 97 ppm by 2100. It is well established that CO₂ fertilization typically stimulates C3 plant photosynthesis and primary productivity in terrestrial ecosystems, basically leading to the increase in plant body size. However, whether the enhanced C uptake under rising CO₂ concentration may increase the dimension of marsh plant in coastal wetlands, has not been well examined through manipulative experiment. The morphology of marsh plant plays critical roles in coastal wetlands because it shields habitats and homes from floods and hurricanes, sustains nests for waterfowls, and supplies nurseries for nektons. To investigate the effects of elevated CO₂ on the morphology of marsh plant, open top chambers (OTC, double the CO₂ concentration in the elevated chambers compared to the ambient chambers) were set up at Smithsonian Global Change Research Wetland (GCREW) in Kirkpatrick Marsh, Rhode River Estuary, Chesapeake Bay. C3 plant shoot dimension, biomass, carbon (C) and nitrogen (N) concentration were measured annually. Here after 30 years CO₂ enrichment we found a significant and 18.5% decrease in the stem leaf area but an increase of 51.9% in stem density of C3 sedge *Schoenoplectus americanus* (Pers.). The CO₂-induced stimulation of sedge productivity and litter accumulation, the depletion of soil N availability, and plant C:N shift all suggest N-limitation of the CO₂ effect. The soil N availability becomes increasingly limiting as the shift of plant C:N may not compensate CO₂ induced N deficiency. Marsh plant trends to allocate more biomass to rhizome and root for nutrient uptake so that the N limitation can be alleviated. The extending rhizome system leads to more tiller recruitment of stems, while the shrinking stem occurs along with the N depletion. Moreover, an increase of 9.6% in stem leaf area of *S. americanus* was found in another 10 years elevated CO₂ plus N addition experiment, suggesting the mitigation of N limitation can reverse the effect of elevated CO₂ on stem dimension. The results from two experiments indicate that the response of marsh plant morphology to elevated CO₂ is regulated by soil N availability and the trade-off between stem dimension and density of marsh plant.

Coastal Wetland Carbon Sequestration in a Warmer Climate

Pat Megonigal, Smithsonian Environmental Research Center
Paul Dijkstra, Northern Arizona University
Matthew Kirwan, Virginia Institute of Marine Sciences
Roy Rich, Smithsonian Environmental Research Center
Peter Thornton, Oak Ridge National Laboratory
Glenn Guntenspergen, US Geologic Survey

Coastal wetlands are global hotspots of carbon storage. Marshes, mangroves, and seagrass meadows account for about half of the total marine soil carbon budget and bury carbon at rates roughly equivalent to terrestrial forests despite occupying just 2.5% of Earth's land area. Such extremely high rates of carbon sequestration are attributed to interactions among three primary factors: high rates of plant production, low rates of decomposition, and sea level rise. As rates of sea level rise accelerate, coastal wetlands have the potential to sequester soil carbon at increasingly rapid rates as long as plants survive flooding and contribute to soil building. Compared to upland soils, the sequestration potential of tidal wetland soils is extremely high because rising sea level increases the potential soil volume over time, and therefore reduces carbon saturation effects typical of upland soils. Coastal wetlands have only recently been recognized as important carbon sinks, and therefore the response of carbon cycling to global change in this ecosystem is virtually unexplored. The future sink strength and carbon stock stability of these systems is uncertain because global change drivers such as temperature and elevated CO₂ perturb the complex biotic and abiotic feedbacks that drive high rates of soil carbon sequestration. Despite the extraordinary leverage these ecosystems exert over the global carbon cycle, the dynamics of coastal wetland carbon pools are not presently represented in earth system models.

Our objectives are to quantify how warming affects the stability of large coastal wetland soil carbon pools, the ability of coastal wetlands to maintain contemporary rates of carbon sequestration, and to quantify interactions between temperature, elevated CO₂ and inundation frequency on soil carbon dynamics. Specifically, we will (i) initiate the first *in situ*, active aboveground and belowground warming experiment in a coastal wetland, and examine the interaction between warming, elevated CO₂ and inundation frequency, (ii) test the overarching hypothesis that warming will increase both plant production and decomposition, but that the net effect will be an increase in soil carbon sequestration rate, (iii) modify a well-established marsh carbon model to incorporate new insights gleaned from the warming experiment, including the impact of warming on productivity and decay, and potential interactions between inundation, warming, and elevated CO₂ that vary with plant species across real-life wetland landscapes. (iv) migrate this refined marsh carbon model into the new wetland-enabled Community Land Model (CLM), producing the first attempt to capture tidal wetland dynamics in a fully prognostic land surface model with coupled water, energy, carbon and nutrient cycles.

The experiment has a gradient design with air and soil warming treatments ranging from 0 to +3.9 °C, to a soil depth of 1 m. Elevated CO₂ will be crossed with temperature at the extremes (0, +3.9). Replicate transects (n=3) will be located in each of two plant communities yielding a plant community treatment that corresponds to changes in inundation across the wetland landscape. The design emphasizes plant and soil biogeochemical measurements that will be used to test and further develop a marsh carbon model. In addition, we will migrate new coastal wetland carbon cycle processes from our refined marsh carbon model into the wetland-enabled CLM framework to evaluate performance of the coastal wetland carbon model in a broader terrestrial ecosystem context, with fully coupled water, energy, carbon, and nutrient cycles.

Title: Extrapolating carbon dynamics of seasonally dry tropical forests across geographic scales and into future climates: improving simulation models with empirical observations

Program: TES

PI: Jennifer Powers, University of Minnesota, powers@umn.edu

Co-Is/Collaborators: Co-I David Medvigy (Princeton), Co-I Forrest Hoffman (ORNL), Co-I Xiaojuan Yang (ORNL), Co-I Bonnie Waring (UMN), Kara Allen (UMN), Xiangtao Xu (Princeton), Annette Trierweiler (Princeton), Camila Pizano (ICESI-Colombia), Beatriz Salgado (Humboldt-Colombia), Juan Dupuy (CICY-Mexico), Catherine Hulshof (U Puerto Rico)

BACKGROUND-- Seasonally dry tropical forests (SDTFs) experience a pronounced dry season lasting 3 to 7 months, and once accounted for approximately 40% of all tropical forest. Dry forests are understudied compared to tropical rainforests, and are poorly represented in earth system models. Thus, it is unknown whether SDTFs are uniquely vulnerable or resilient to global environmental changes including climate change and nitrogen deposition. We hypothesize that the responses of SDTFs to global change depend critically on belowground processes, but we lack empirical data to verify this.

OBJECTIVES—The objectives of this project are to quantify how above- and belowground processes mediate the responses of SDTF carbon dynamics to environmental change, and incorporate that understanding into two state-of-the-art models, ED2 and ACME. To do so, we are using an interdisciplinary approach that integrates: 1) field observations of ecosystem processes and plant functional traits across a range of dry forest sites in Costa Rica, Mexico, Puerto Rico, and Colombia, 2) forest-scale experiments that manipulate water and nutrient availability in Costa Rica, and 3) model simulations that quantify sensitivity of ecosystem carbon cycling to external forcings. Ultimately, our combined measurement and modeling approach will elucidate controls on C cycling in SDTFs and yield improved models for the global change research community.

RESULTS AND PROGRESS-- Empirical results We established a large-scale factorial nitrogen (N) and phosphorus (P) fertilization experiment in Costa Rica. To date, we have found that belowground processes respond rapidly to fertilization. Soil respiration fluxes decreased in +N, +P and N+P relative to unfertilized plots, whereas root productivity increased in all fertilized plots. Mycorrhizal colonization decreased dramatically in the N+P treatment only, while nodulation more than tripled in the +P treatment. Ongoing work includes a large-scale throughfall exclusion experiment and observations of ecosystem processes across the network of sites. ED2 results The Ecosystem Demography model 2 (ED2) was updated with a trait-driven mechanistic plant hydraulic module and a new drought-phenology scheme. Four plant functional types were parameterized based on meta-analysis of plant hydraulic traits. Simulations from both the original and the updated ED2 were evaluated against 5 years of field data from a Costa Rican SDTF site and remote-sensing data over Central America. The updated model generated realistic simulations of tree diameter growth, litterfall, phenology and the variations of these quantities among functional groups. Overall, we find that mechanistic incorporation of plant hydraulic traits is necessary for simulating spatio-temporal patterns of vegetation dynamics in SDTFs in vegetation models. We have also developed a new, stoichiometrically-based formulation of plant nutrient limitation. This formulation includes symbiotic nitrogen fixation, plant-mycorrhizal interactions, and phosphatase exudation. Work is ongoing to parameterize both ED2 and ACME with data collected from the field sites.

An observational constraint on stomatal function in forests: evaluating coupled carbon and water vapor exchange with carbon isotopes in the Community Land Model (CLM 4.5)

B. Raczka, H. Duarte, C. Koven, D. Ricciuto, P. Thornton, J. C. Lin, D. R. Bowling

Land surface models are useful tools to quantify contemporary and future climate impact on terrestrial carbon cycle processes, provided they can be appropriately constrained and tested with observations. Stable carbon isotopes of CO₂ offer the potential to improve model representation of the coupled carbon and water cycles because they are strongly influenced by stomatal function. Recently a representation of stable carbon isotope discrimination was incorporated into the Community Land Model component of the Community Earth System Model. Here, we tested the model's capability to simulate whole-forest isotope discrimination in a subalpine conifer forest at Niwot Ridge, Colorado, USA. We implemented a V_{cmax} seasonally-varying model formulation that optimized net CO₂ carbon exchange, latent heat exchange and biomass relative to observations. The model accurately simulated observed $\delta^{13}\text{C}$ of needle and stem tissue, but underestimated the $\delta^{13}\text{C}$ of bulk soil carbon by 1-2 ‰. The model overestimated the (2006-2012) average Δ_{canopy} relative to prior data-based estimates by 5-6 ‰. The amplitude of the average seasonal cycle of Δ_{canopy} (i.e. higher in spring/fall as compared to summer) was correctly modeled but only with an alternative formulation for nitrogen limitation. The model attributed most of the seasonal variation in discrimination to the net assimilation rate (A_n), whereas inter-annual variation in Δ_{canopy} during the summer months was driven by stomatal response to vapor pressure deficit. Soil moisture did not influence modeled Δ_{canopy} . Model results indicated that there has been an increase in both photosynthetic discrimination and water use efficiency (WUE, 10%) since 1850 as a result of CO₂ fertilization, under constant climate conditions. This increasing trend in discrimination is counter to established relationships between discrimination and WUE. The isotope observations used here to constrain CLM suggest 1) the parameterization for stomatal conductance was too large and should be reduced via stomatal slope adjustments and 2) the default approach to representing nutrient limitation was not capable of reproducing observed trends in discrimination. These findings demonstrate that isotope observations can bring important information related to stomata function driven by environmental stress from VPD and nitrogen limitation.

The Role of Phenolic Compounds, Aromatics and Black Carbon Controls on Decomposition, GHG losses in Peatlands Along a Latitudinal Gradient from Minnesota to Panama

Curtis J. Richardson^a, H. Wang^a, S. Hodgkins^c, N. Flanagan^a, B. Cooper^b, J. Tian^a, M. Ho^a, and J. Chanton^c

^a *Duke University Wetland Ctr., Nicholas School of the Environment, Durham, NC 27708, USA*
curtr@duke.edu

^b *Department of Chemistry and Biogeochemistry, Florida State University, Tallahassee, FL, 32306, USA*

^c *Department of Earth, Ocean and Atmospheric Science, Florida State University, Tallahassee, FL, 32306, USA*

Peatlands have persisted through changing climate over millennia and continue to accrete peat in many globally warmer areas even under accelerated climate driven conditions of drought, warming and fire. Our main hypothesis is that a dual control or “latch mechanism” reduces decomposition in shrub/tree communities in subtropical and tropical peatlands due to (1) higher production of polyphenol and aromatic compounds than found in northern *Sphagnum/Carex* communities, and (2) the buildup of recalcitrant organic matter (black carbon, BC) by light fire in the native-fire-adapted communities leads to a reduction in microbial decay of peat. Here, linking intensive biological and chemical analysis in a series of field and microcosm experiments along our north to south bog gradient from Minnesota to Panama we show how previously unrecognized interactions between these dual mechanisms regulate C sequestration in peatlands. Key findings to-date include (1) a N to S gradient of phenolics exists with NC Pocosin peats having the highest concentrations due to the dominance of high-phenolic shrubs; (2) Peat soil in Pocosins with fire-adapted shrubs also contained the highest BC with the highest hydrophobicity; (3) Fungal communities principally responsible for lignin decomposition were significantly different between northern and Pocosins. Archaeorhizomycetes dominante in Pocosins (11%~52%), while comprising < 1% in northern peatlands, which indicates that long-term drought/fire adapted shrubs may culture fungi with low decomposition ability; (4) Using FTIR and ¹³C NMR on solid soil samples, we observed increased aromaticity and lower carbohydrate content at lower latitude sites, which indicate that peat in warmer climates lose carbohydrates more rapidly or initially contain lower carbohydrates with higher aromaticity; (5) DOC results obtained with FT-ICR mass spectrometry and EEMS fluorescence spectroscopy indicated lower aromaticity and lower molecular weight compounds at Everglades sites consistent with greater microbial production of the DOC; (6) Recent prescribed fires at the Pocosins strongly decreased carbohydrate content but exposing soil directly to sunlight stimulated CO₂ production by increasing soil temperature. Such priming effects may disappear later, as our in-lab heating experiment shows lower CO₂ emission from burned peat after an initial pulse; (7) Fungal communities in Pocosins were most diverse shortly after the prescribed burn but declined over time. Next year based on current results, we will conduct more in-depth microbial, biological and chemical analysis to explore the potential effects of climate change, like drought and warming, on peat/litter accumulation in boreal, temperate and tropical peatlands, and will further test a phenol/black carbon model.

Canopy water use efficiency before, during and after gypsy moth attack in an upland forest in the New Jersey Pine Barrens

Karina VR Schäfer, Diane Radwanski, Tomer Duman, Kenneth L Clark

The New Jersey Pine Barrens are a fire adapted, ecosystem in central-south New Jersey. The soil is sandy, and thus well-drained and nutrient poor. Due to fire suppression and thus natural succession, the upland forest consists approximately to one third of oak/pine forests that are susceptible to gypsy moth infestation and drought. This upland oak/pine stand experienced a gypsy moth infestation in 2007 and a very severe drought in 2010 that resulted in a 30% mortality of larger oak trees. Such events cause changes in water, nutrient and light availability, which in turn affect the canopy water use efficiency and carbon uptake. Here, we present sap flow measurements over ten years from 2005 to 2014 with the heat balance and heat dissipation method and leaf level photosynthesis measurements from 2006, 2010, and 2012-2014 using a Licor 6400 XT. Parallel eddy covariance measurements were used to estimate evapotranspiration over the 2004 to 2014 time period. Applying these measurements with the Canopy Conductance Constrained Carbon Assimilation model (4CA), we demonstrate the changes in canopy water use efficiency over this ten-year period.

Over the ten-year period, canopy water use declined due to mortality and has as of yet, not rebound to pre-defoliation levels. However, water use has not proportionally dropped to mortality, due to compensation of surviving trees, mostly white oak species and pines, whereby red oak species declined. Moreover, water use efficiency dropped throughout the study period by approximately 20% mostly due to higher water availability of the surviving trees compared to commensurate carbon uptake. The photosynthetic capacity, however, has increased by 25% from 2006 to 2013, mostly due to higher light availability and partially higher nitrogen content in the leaves. Thus, although mortality and defoliation increase availability of water and light, the surviving population does not increase their water use efficiency, but rather shift to a more wasteful water resource management. Eddy flux measurements indicate that while evapotranspiration has approached pre-disturbance levels, the rate of carbon sequestration has not recovered yet. Overall, after several years this forest has still not recovered to pre-defoliation levels of canopy water use efficiencies and canopy carbon uptake.

Project title: Carbon cycle dynamics in Oregon's urban-suburban-forested-agricultural landscapes

Andres Schmidt (presenter), Beverly E. Law (PI), Chris Still, Thomas Hilker

Department of Forest Ecosystems and Society, Oregon State University, Corvallis, OR 97331

Abstract:

The combined effects of changes in land-use and land cover (LULC) and climate on carbon and water cycling need to be assessed at regional scales. LULC changes over time have many drivers such as expanding urban areas, exploration of new agricultural areas due to overused natural resources of current agricultural areas (e.g. degraded soil), economical reasons, or policy changes that encourage the use of alternative energy resources. Our study is focused on the effects of conversion of semi-arid sagebrush and Willamette Valley agricultural crops to bioenergy production on carbon, water and energy cycling, and resulting heating or cooling effects. Our project focusses on Oregon, where agricultural crops, significant forest area, and urban expansion are coupled with a strong spatial climate gradient that allows us to examine influences on carbon sequestration by the terrestrial biosphere. Our inverse modeling results with the CO₂ tower observations showed that CLM4.5, parameterized by species groups instead of standard PFTs, underestimated NEE in the highly productive western Douglas fir forests by more than 50%. Further diagnosis suggests the soils data inputs do not capture the high nitrogen and soil water holding capacity of the highly productive forests in the Coast Range. By integrating remote sensing LULC data, eddy covariance data from flux sites, tall tower CO₂ observations, biomass estimates from field samples, and the improved CLM4.5, we predict current and future statewide carbon sequestration with unprecedented accuracy. Using inventories and tower flux data, we determined the effect of conversion of hay and grass seed cropland (323,200 ha) to hybrid poplar and found the state NEP increased from 4 TgCO₂ per year to 13 TgCO₂ per year for that area. The last coal power plant in the state (Boardman) is in the process of switching from coal combustion to biofuel burning to meet the state's goal for the reduction of greenhouse gas emissions. Our results show that the 7816 tons of biomass per day to keep the 518 MW power plant running at base load would amount to 35,000 hectares of poplar per year under current climate conditions. The improved CLM4.5 model will be used to evaluate the impacts of this land use change on the net ecosystem carbon balance (NECB) and net emissions to the atmosphere under future climate conditions. We will also examine water vapor feedback effects on the energy budget.

TES Program

The impact of permafrost carbon loss on the carbon balance of an experimentally warmed tundra ecosystem

Authors: E.A.G. Schuur¹, E. Pegoraro¹, M. Mauritz¹, C. Schaedel¹, R. Bracho², J. Hutchings², V. Salmon², E. Webb², S.M. Natali³, K. Coe⁴, Junyi Liang⁵, Yiqi Luo⁵, Caitlin Pries Hicks⁶, Charlie Koven⁶.

¹Northern Arizona University; ²University of Florida; ³Woods Hole Research Center; ⁴Cornell University; ⁵Oklahoma University; ⁶Lawrence Berkeley National Laboratory;

New estimates place 1330-1580 billion tons of soil carbon in the northern circumpolar permafrost zone, more than twice as much carbon than in the atmosphere. Permafrost thaw and the microbial decomposition of previously frozen organic carbon is considered one of the most likely positive feedbacks from terrestrial ecosystems to the atmosphere in a warmer world. Understanding the magnitude, rate, and form of greenhouse gas release to the atmosphere is crucial for predicting the strength and timing of this carbon cycle feedback to a warming climate. Here we report results from eight years of an ecosystem warming manipulation—the Carbon in Permafrost Experimental Heating Research (CiPEHR) project—where we increased air and soil temperature, and degraded the surface permafrost. We used snow fences coupled with spring snow removal to increase deep soil temperatures and thaw depth (soil warming) and open top chambers to increase growing season air temperatures (air warming). The soil warming treatment has successfully warmed soils by 2-3°C in winter, has increased growing-season depth of ground thaw by up to 25-50%, and has degraded an increasing amount of surface permafrost each year of the project. The treatment has led to the development of continuously thawed soil layers deep within the profile that remain above zero even during the cold winter. Surface subsidence as a result of permafrost thaw previously had increased surface soil moisture and reduced the distance from the soil surface to the water table. These unfrozen layers have led to threshold changes in surface moisture that is normally perched on the permafrost table, with thaw breakthroughs drying the soil surface, at least periodically, during the growing season. We showed that experimental warming that caused permafrost degradation led to a two-fold increase in carbon uptake by the ecosystem during the growing season. Warming also enhanced growing season and winter respiration, which, in part, offset growing season carbon gains. This was in part due to more old carbon released by soil warming both during the growing season and the winter. Assimilating experimental data into an ecosystem model indicated that parameter adjustment was needed for the model to simulate carbon cycle dynamics under experimental warming. In particular, parameters for light use, gross primary production allocation, as well as transfer coefficients from litter to soil pools showed the greatest change, suggesting that there was acclimation in ecosystem behaviour in response to warming.

Using a spatially-distributed hydrologic biogeochemistry model to study the spatial variation of carbon processes in a Critical Zone Observatory

Yuning Shi¹, David Eissenstat¹, Kenneth Davis^{2,3}, Jason Kaye¹

Forest carbon processes are affected by soil moisture, soil temperature, Nitrogen availability and solar radiation. Most of the current biogeochemical models are 1-D and represent one point in space. Therefore they can neither resolve topographically driven hill-slope soil moisture patterns, nor simulate the nonlinear effects of soil moisture on carbon processes. A spatially-distributed ecosystem-hydrologic model, Flux-PIHM-BGC, has been developed by coupling the Biome-BGC (BBGC) model with a coupled physically-based land surface hydrologic model, Flux-PIHM. Flux-PIHM incorporates a land-surface scheme (adapted from the Noah land surface model) into the Penn State Integrated Hydrologic Model (PIHM). Because PIHM is capable of simulating lateral water flow and deep groundwater, Flux-PIHM is able to represent the link between groundwater and the surface energy balance, as well as the land surface heterogeneities caused by topography.

Flux-PIHM-BGC model was tested at the Susquehanna/Shale Hills critical zone observatory (SSHCZO). The abundant observations at the SSHCZO, including eddy covariance fluxes, soil moisture, groundwater level, sap flux, stream discharge, litterfall, leaf area index, aboveground carbon stock, and soil carbon efflux, provided an ideal test bed for the coupled model. Model results show that the vegetation and soil

carbon distribution is primarily constrained by N availability (affected by N transport driven by topography), and also constrained by solar radiation and root zone soil moisture. The predicted vegetation and soil carbon distribution generally agrees with the macro pattern observed within the watershed. The coupled ecosystem-hydrologic model provides an important tool to study the impact of topography on watershed C processes.

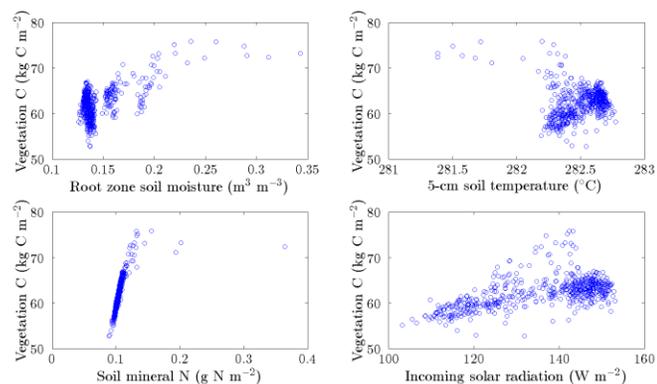


Figure 1 Annual average vegetation carbon plotted as functions of root zone soil moisture, soil temperature, soil mineral N, and incoming solar radiation from Flux-PIHM-BGC simulation. Each point represent on grid in the Shale Hills watershed model domain.

¹ Department of Ecosystem Science and Management, The Pennsylvania State University.

² Department of Meteorology, The Pennsylvania State University.

³ Earth and Environmental Systems Institute, The Pennsylvania State University.

Soil carbon pools are much larger than most other carbon pools on the planet. Fine root turnover represents the most significant mode of carbon flux from plants into these pools, outstripping the role of leaves and other aboveground litter. In addition to the large scale at which fine roots are contributing to soil carbon pools, there is experimental evidence that carbon derived from dead root biomass is more likely to remain in soil carbon pools than carbon derived from aboveground litter such as that from leaves. Unfortunately, fine root senescence, a critical component of belowground biology is particularly understudied. The control of senescence in fine roots, and the fate of elements and organic molecules they contain during root death, still remains largely unknown. In addition to its contribution to basic biological understanding, better understanding fine root senescence should reduce uncertainty associated with global climate models; including re-uptake of materials in dying leaves into these models has already been shown to increase their accuracy. It is very likely that including the consequences of root senescence will have similar benefits to the accuracy of these models.

We are using experimental manipulations to impose fine root senescence in *Pinus taeda* in a field setting. These include two girdling manipulations and a third control. Each treatment is applied to 4th order roots and the effects of girdling will be assessed on fine roots distal to the site of manipulation. The signal resulting from these treatments will include changes in anatomy, chemical content, and gene expression through time. The impacts of these treatments on the internal anatomy of fine roots and the loss of stored carbohydrates in the form of starch granules will be examined using classical histological approaches. The abundance and identity of C and N containing compounds will be assessed using laser-ablation GC. Finally we will examine differential gene expression profiles among treatments.

To track fine roots through time and access them for manipulations in the field, we have installed 100 30x30cm plastic "root windows" at a site in coastal SC. These windows were installed in summer 2015 and nearly all have been colonized by *P. taeda* roots by winter 2016. In January 2016 we conducted girdling trials experiments and in early February we collected the treated roots for sectioning and anatomical analysis. We are performing the full experimental manipulations including all treatments across replicated root windows in early March, 2016.

Net bVOC emissions from a mixed hardwood forest floor: Importance of species composition and belowground processes in driving seasonal dynamics

Award Number: DE-SC0010845

TES program poster abstract

PI: Amy M. Trowbridge

Authors: Amy M. Trowbridge, Luke Jacobs, Paul C. Stoy, Philip Stevens, Richard P. Phillips

Affiliation: Montana State University Department of Land Resources and Environmental Sciences

Email: amy.trowbridge@montana.edu

Our understanding of the sources of and controls over bVOC fluxes from terrestrial ecosystems remains incomplete. Namely, leaf litter and soils have recently been determined to be an important component of ecosystem bVOC source sink dynamics, yet emission models have yet to incorporate processes occurring at or below the soil surface, likely due to the complex nature of these interactions and general lack of data. The aim of our project is to quantify the mechanisms controlling soil bVOC uptake and emissions from a mixed hardwood forest – the Morgan Monroe State Forest Ameriflux research site in Indiana – within the context of plant-mycorrhizal interactions, tree species composition, and environmental and physical factors.

Data from our monthly field measurements of soil collars during the beginning and end of the 2014 growing season suggest that forest soils inhabited by tree species associated with arbuscular (AM) and ectomycorrhizal (ECM) fungi are a net bVOC source early in the growing season following leaf-out. As the season progressed into the fall, AM plots remained a small source yet ECM plots became a significant bVOC sink. As the leaves began to senesce and more litter accumulated on the forest floor, ECM plots once again became a bVOC source of the same magnitude observed in May with no change in emissions from AM-plots. Thus, in the fall when the major ecosystem bVOC source from the canopy is absent, the forest floor provides another source of VOCs whose magnitude and quality reflect differences in relative tree species composition, and thus, litter quality, decomposition, and the associated microbial communities.

We are currently analyzing these data to quantify relationships between the aforementioned variables observed in these plots over time. During 2015, we measured soil and litter bVOC flux at a higher temporal frequency during the dynamic senescence period. We coupled these soil measurements with bVOC concentration profiles within the canopy to investigate bVOC transport and the relative importance of soil fluxes at the ecosystem level. Initial data indicates that recently senesced leaf litter produces a large flux of bVOC, and that soils serve as a sink to a fraction of these emissions. Furthermore, this effect is differentiable between soils and litter associated with AM and ECM mycorrhizal fungi, providing a potentially useful framework in which to model bVOC emissions over time in deciduous hardwood forests.

Tracking the fate of Arctic carbon: will shrub expansion result in a loss of soil carbon?

Laurel Lynch, Megan Machmuller, Francesca Cotrufo, Matthew Wallenstein

Northern circumpolar soils cover 16% of the global land surface area, yet they account for nearly 50% of the estimated terrestrial organic carbon (C) pool. Unprecedented rates of warming may convert the Arctic from a net sink to net source of atmospheric C if temperature is the dominant mechanism of soil organic matter (SOM) accrual and retention. Additionally, climate projections indicate an increase in the abundance of woody shrubs, potentially increasing the total amount of labile C added to the system. Our ability to predict the response of Arctic C cycling is limited by uncertainties in our understanding of the processes that may counteract or enhance SOM loss. Our research objective is to improve our mechanistic understanding of the effects of labile C inputs into Arctic soils.

In July 2014 we added ^{13}C -glucose, simulating root exudates, to soils dominated by two dominant Arctic vegetation species: *Betula nana*, a vigorously expanding woody dwarf birch species, and *Eriophorum vaginatum*, a ubiquitous tussock-forming sedge. Stable isotopes allow us to partition the fate of ^{13}C -glucose among various pools. We measured $^{13}\text{CO}_2$ efflux in situ with a cavity ringdown spectrometer and analyzed a suite of biogeochemical variables on harvested soils. We also tracked ^{13}C -glucose incorporation into microbial biomass, transformation to DOM, and stabilization within the bulk soil. This experiment was repeated during senescence (September) and spring thaw (May 2015) to assess seasonal influences on substrate use dynamics. An additional subset of collars were labeled in July and measured in September and May to track long-term changes in soil C cycling following substrate input.

Our results indicate greater respiration and ^{13}C -glucose utilization under *E. vaginatum* with no short-term native SOM loss under either vegetation type. Overall, only ~10% of ^{13}C -glucose was measured in CO_2 efflux, and no priming of the microbial community was observed beneath either vegetation type. Low overall incorporation of ^{13}C in microbial biomass indicates either low substrate utilization or fast substrate cycling through the microbial loop and excretion of metabolic byproducts to the bulk soil. Particularly high ^{13}C enrichment of bulk soil beneath *B. nana*, combined with our $^{13}\text{CO}_2$ efflux results, suggest new inputs of labile carbon will not result in an immediate destabilization of native soil organic matter. Our findings indicate the Arctic may be more resilient to climate change than expected.

Benchmarking and improving microbial-explicit soil biogeochemistry models

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Will Wieder^{1,2}, Melannie Hartman², Ben Sulman³, Steve Allison⁴, Jim Randerson⁴, Hua Wally Xie⁴, Rich Phillips⁵, Adrienne Keller, Matthew Craig, & Stuart Grandy⁶

Earth system models that are designed to project future carbon (C) cycle – climate feedbacks exhibit notably poor representation of soil biogeochemical processes and generate highly uncertain projections about the fate of the largest terrestrial C pool on Earth. Given these shortcomings there has been intense interest in soil biogeochemical model development, but parallel efforts to create the analytical tools to characterize, improve and benchmark these models have thus far lagged behind. A long-term goal of this work is to develop a framework to compare, evaluate and improve the process-level representation of soil biogeochemical models that could be applied in global land surface models. Here, we present a newly developed global model test bed that is built on the Carnegie Ames Stanford Approach model (CASA-CNP) that can rapidly integrate different soil biogeochemical models that are forced with consistent driver datasets. We focus on evaluation of two microbial explicit soil biogeochemical models that function at global scales: the MIMICs and CORPSE models. Using the global model test bed coupled to MIMICs and CORPSE we quantify the uncertainty in potential C cycle – climate feedbacks that may be expected with these microbial explicit models, compared with a conventional first-order, linear model. By removing confounding variation of climate and vegetation drivers, our model test bed allows us to isolate key differences among different soil model structure and parameterizations that can be evaluated with further study. Specifically, the global test bed also identifies key parameters that can be estimated using cross-site observations. In global simulations model results are evaluated with steady state litter, microbial biomass, and soil C pools and benchmarked against independent globally gridded data products.

Affiliations & email addresses:

¹University of Colorado, Boulder, wieder@colorado.edu

²National Center for Atmospheric Research, Melannie.Hartman@colostate.edu

³Princeton University, bsulman@princeton.edu

⁴University of California, Irvine, allisons@uci.edu, jranders@uci.edu, xiehw@uci.edu

⁵Indiana University, rpp6@indiana.edu, kellerab@indiana.edu, maecraig@uemail.iu.edu

⁶University of New Hampshire, Stuart.Grandy@unh.edu

SFA - SBR ABSTRACTS

IDEAS ABSTRACTS

Assessing groundwater surface water interactions using an integrated hydrologic model of the Continental US

Condon, L.E., I.E.M. de Graaf, R.M. Maxwell

We evaluate groundwater surface water interactions using the first high-resolution integrated hydrologic model of the continental US developed for Use Case 3 of the Interoperable Design of Extreme-scale Application Software (IDEAS) project. Spatial patterns in the physical controls of groundwater depth and flux are assessed using a steady state predevelopment simulation. Results illustrate clear multi scale behavior and regional shifts in the relative control of topography, geology and climate on groundwater. In agreement with previous studies, this simulation demonstrates relatively greater topographic control and more significant groundwater exchanges along streams in the arid west than in the humid east. Dynamic interactions from the groundwater to the land surface are simulated using ParFlow-CLM for a one-year transient simulation spanning water year 1985. Model outputs are validated against more than 30,000 groundwater and surface water gauges with available observations for the simulation period. We use the combination of high-resolution (1 km²) outputs covering a large spatial extent (~6.3 million km²) to characterize groundwater surface water exchanges across a broad range of hydroclimatic settings and spatial scales.

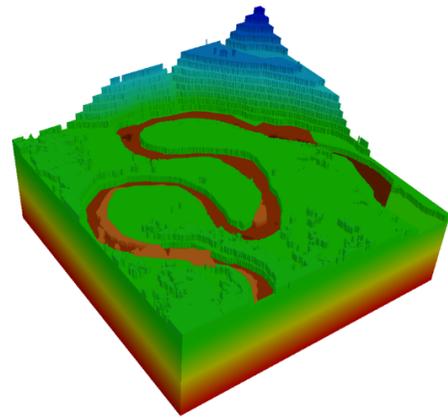
Building from the existing CONUS model, we are also working with an interdisciplinary team to expand the domain from coast-to-coast and increase the spatial resolution to 250 m². Information on aquifer characteristics, such as thickness and conductivities, was not previously available at this level of detail and is needed to improve model performance. As a next step towards the development of a hyper-resolution model for the US, we developed the first US aquifer map including information on aquifer thicknesses and spatial distribution of alluvial aquifer systems and consolidated aquifers. The aquifer map is based on a combination of USGS data on spatial distribution and reported thicknesses of the upper alluvial aquifers, and an estimate of local river valley thicknesses, mainly based on terrain attributes. Consolidated aquifer thicknesses were estimated assuming declining conductivities with increasing depth. The new aquifer map will be incorporated into the expanded ParFlow-CLM model and used to evaluate the impacts of aquifer parameterization on simulated groundwater surface water interactions. Overall, the progress made in Use Case 3 highlights advances in large scale integrated modeling and the potential for such tools to improve our understanding hydrologic interactions and sensitiveness at unprecedented scales.

Testing Code Interoperability and Productivity on Modeling Integrated Surface-Subsurface Water Flow and Biogeochemical Cycling in the Hyporheic Zone – IDEAS Use Case 1

Dipankar Dwivedi¹, Carl Steefel¹, Erica Woodburn¹, David Moulton², Ethan Coon², Lauren Foster³, Reed Maxwell³

¹Lawrence Berkeley National Laboratory, ²Los Alamos National Laboratory, ³Colorado School of Mines

The overarching goal of Interoperable Design of Extreme-scale Application Software (IDEAS) is to leverage enhancements in software library interoperability and design to enable a new level of spatial and time resolution as well as process fidelity in the modeling of multi-scale terrestrial ecosystems. To demonstrate the approach, the Use Case 1 of IDEAS effort focuses on the development of a set of benchmark problems that leverage interoperable software components to investigate the roles of integrated surface-subsurface water flow, transport, and biogeochemical cycling in the East River Watershed, Colorado. The shorter-term objective is to understand the effects of hyporheic zone exchange in tight meanders of the lower East River floodplain on nutrient (especially nitrogen), carbon, and metal riverine fluxes from the greater watershed. The longer term objective is to develop an approach for upscaling results to larger domain sizes (e.g., 10 km by 10 km). The initial benchmarks will make use of high resolution LIDAR and bathymetric data to investigate productivity issues on an approximately 175 meter by 175 meter horizontal by 25 meter vertical modeling domain with the lateral grid resolution of 0.5 meters. The benchmark simulations are being developed using the codes ParFlow, Amanzi-ATS, and PFLOTRAN, which provide slightly contrasting modeling approaches for quantifying integrated hydrological and biogeochemical response. ParFlow relies on tightly coupled surface and subsurface water simulations and terrain stepping treatment of topography on a fixed grid, Amanzi-ATS uses variable resolution unstructured grids to capture important interfaces and gradients, while PFLOTRAN will soon have the capability for integrated surface and subsurface water flow. These codes take advantage of improvements in interoperability by accessing biogeochemistry through the Alquimia interface.



3-D modeling domain for lower East River meanders. Domain size is approximately 175m by 175m by 25m with a lateral grid resolution of 0.5 m.

We are also beginning the development of an East River watershed scale simulation based on an approximately 10 km by 10 km modeling domain using the same 0.5 meter resolution LIDAR data that will require exascale computing platforms. This will test the ability of the codes to make use of the high resolution topography on a larger watershed-scale domain. These will also be compared with the results of 10 meter resolution simulations over the same domain.

Interoperable software for integrated watershed scale models

Jeffrey Johnson¹, Sergi Molins¹, Ethan Coon², Reed Maxwell³

¹Lawrence Berkeley National Laboratory, Berkeley, CA

²Los Alamos National Laboratory, Los Alamos, NM

³Colorado School of Mines, Golden CO

As our models become more elaborate and move toward multiscale representations, it is more clear than ever that we need the ability to combine different computational processes and algorithms in a sensible and interoperable fashion. Proponents of modern software engineering argue that this interoperability can be achieved by wrapping existing software in modular interfaces, but the design of these interfaces must be simple enough for practitioners to use and relevant to their needs. The Interoperable Design of Extreme-scale Software Applications (IDEAS) project is exploring this challenging problem in a few different settings. We examine the interface in the Community Land Model (CLM) used by ParFlow, which is intended to be released as a reusable software component. In this context, we discuss the development of guidelines for interfaces between integrated hydrology models and land models. We also describe ongoing work on Alquimia, an interoperable interface designed to provide biogeochemical processes to flow/transport models. The Alquimia interface now supports fully implicit integration of reaction terms, augmenting its previous operator-split treatment. This new feature allows users of Alquimia to study the effects of different methods for coupling transport and reaction processes, and simplifies the process of benchmarking. Finally, we outline ongoing efforts to characterize and define extensible interfaces for other processes and process couplings commonly present in modeling across BER.

Interoperable Design of Extreme-scale Application Software (IDEAS): Software development methodologies that enhance scientific productivity

M. Heroux,¹ L. C. McInnes,² J. D. Moulton,³ D. Bernholdt,⁴ H. Johansen,⁵ and the IDEAS team

While emerging extreme-scale computers provide unprecedented resources for scientific discovery, the community faces daunting productivity challenges due to the complexities of multiphysics, multiscale applications and evolving computer architectures. The IDEAS Scientific Software Productivity Project (<https://ideas-productivity.org>) is working to increase software development productivity—a key aspect of overall scientific productivity—through an interdisciplinary and agile approach that centers on adapting modern software engineering tools, practices, and processes to build a flexible scientific software ecosystem. This poster highlights work in four focus areas.

Use Cases: Three important BER use cases drive our work: climate impacts on the upper Colorado river system; hydrology and soil carbon dynamics of the Arctic tundra; and hydrologic, land surface, and atmospheric process coupling over the contiguous U.S. Recent use-case advances include expanded testing and numerical library usage—critical as we build a software ecosystem that enables application scientists to focus on their areas of expertise while easily employing cutting-edge external software. See four IDEAS use-case posters led by J. Johnson, C. Steefel, S. Painter, and L. Condon.

xSDK: A central IDEAS activity is development of an [Extreme-scale Scientific Software Development Kit \(xSDK\)](#) — a collection of related and complementary software elements that provide the building blocks, tools, models, processes, and related artifacts for rapid and efficient development of high-quality applications. The first release of the xSDK in early 2016 will include four numerical libraries ([hypr](#), [PETSc](#), [SuperLU](#), and [Trilinos](#)) and the [Alquimia](#) geochemistry interface. Draft [xSDK package compliance standards](#) and [xSDK standard configure and CMake options](#) help to address challenges in interoperability and sustainability of software developed by diverse groups.

HowTo: To help cultivate best practices and processes for improved scientific software development, we have written concise [WhatIs and HowTo documents](#) that characterize important software topics in "bite-sized" levels of detail that enable software teams to consider improvements at a small but impactful scale. Topics include software configuration, testing, documentation, performance portability, and interoperability.

Outreach: The final piece of IDEAS is outreach and collaboration with the broader computational science and engineering (CSE) community, which is also facing similar productivity challenges. We are developing training materials in collaboration with ALCF, NERSC, and OLCF. We also have established the CSE Software Forum (<https://cse-software.org>) as an umbrella for a community of interest/practice in software engineering for CSE on high-performance computers.

¹ Sandia National Laboratories

² Argonne National Laboratory

³ Los Alamos National Laboratory

⁴ Oak Ridge National Laboratory

⁵ Lawrence Berkeley National Laboratory

A multiscale strategy for process-rich, microtopography-aware simulations of thermal hydrology in polygonal tundra

Scott L. Painter¹, Ethan T. Coon², Ahmad Jan¹, J. David Moulton³

¹Climate Change Science Institute and Environmental Sciences Division, Oak Ridge National Laboratory

²Computational Earth Sciences Group, Los Alamos National Laboratory

³Applied Mathematics and Plasma Physics, Los Alamos National Laboratory

The use of simulations to advance environmental systems science is most effective when insights about the system behavior can be exploited to design computationally effective modeling strategies. However, limitations of current tools often make it difficult to express those thoughtful approximations in simulation software. The Interoperable Design of Extreme-scale Application Software (IDEAS) project is addressing this barrier to productivity using a novel strategy for simulating the thermal hydrology of thawing polygonal tundra as a use case. Simulating the soil thermal hydrology system in degrading carbon-rich permafrost regions is challenging because of strong coupling among thermal and hydrologic processes, the important role of organized microtopography in controlling water flows, strong coupling between the surface and subsurface, and the potential for topographic changes as ground ice melts (e.g. Painter et al. 2013). Motivated by results of fine-scale simulations and in collaboration with the Next Generation Ecosystem Experiments-Arctic (NGEE-Arctic) project, we have designed a computationally tractable strategy that uses individual ice-wedge polygons as the horizontal discretization of the landscape. The independent subsurface columns resulting from that discretization are then coupled indirectly through an overland flow system using a subgrid model to represent the effects of subgrid microtopography on surface flow. Simulations that include thaw-induced subsidence become tractable in this framework because the subsurface thermal hydrology and deformation processes are represented on independent one-dimensional columns, which avoids issues of poor mesh quality that can result from representing dynamic topography in a three-dimensional model. The capability is being implemented in the ATS simulator and will be used by the NGEE-Arctic project to simulate the evolution of polygonal tundra in a changing climate. In addition, the mixed-dimensional spatial structure has broader applicability in watershed modeling. Managing the multiple meshes and multiple process representations in these intuitively appealing mixed-dimensional simulations is a significant software challenge. As part of the IDEAS project's broader goal of enabling a "virtual ecosystem" of composable software components, this Use Case explores how a configurable model coupling system (Coon et al. 2016) can enable this class of mixed-dimensional model.

Painter SL, Moulton JD, Wilson CJ. 2013. Modeling challenges for predicting hydrologic response to degrading permafrost. *Hydrogeology Journal*. 21(1):221-224.

Coon, ET, Moulton, JD, Painter, SL. 2016. Managing complexity in simulations of land surface and near-surface processes, *Environmental Modelling & Software*, Volume 78, April 2016, Pages 134-149, <http://dx.doi.org/10.1016/j.envsoft.2015.12.017>.

ANL ABSTRACTS

The effect of surfaces and ligands on the reduction and reoxidation reactions of U studied in mixed-batch reactors and flow-through columns

SBR - ANL SFA (Laboratory Research Manager: Robin Graham)

M. Boyanov (mboyanov@ice.bas.bg),^{1,2} D. Latta,^{1,3} M. Scherer,³ Y.Liu,⁴ C. Liu,⁴ B. Mishra,^{1,5} E. O'Loughlin,¹ K. Kemner¹

1. Biosciences Division, Argonne National Laboratory; 2. Institute of Chemical Engineering, Bulgarian Academy of Sciences; 3. Department of Civil and Environmental Engineering, The University of Iowa; 4. Pacific Northwest National Laboratory; 5. Department of Physics, Illinois Institute of Technology.

The speciation of uranium (U) is an important control on its mobility in natural systems. Factors such as the valence state and the molecular-scale environment of U influence its solubility and its susceptibility to leaching by groundwater. Subsurface systems contain a host of minerals, bacteria, and dissolved ligands; the interaction between them and U needs to be understood so appropriate reactions can be included in the Reactive Transport Models (RTMs) used to predict contaminant migration and to inform policy decisions.

The Argonne Subsurface SFA is continuing to provide the molecular-level understanding of the processes needed for the development of RTMs. Here, we study the transformations of U caused by changes in redox conditions that may result from a seasonal influx of organic matter or oxidized groundwater. We have shown previously that the precipitation of mononuclear U^{IV} in biostimulated systems is caused by the presence of phosphate in the medium. The reoxidation behavior of such U^{IV}-phosphate species is relatively unknown compared to uraninite. Using synchrotron x-ray spectroscopy we find that U^{IV}-phosphate oxidizes to U^{VI} at similar rates as uraninite. However, when ubiquitous ions such as calcium and phosphate are present in the groundwater the transformation pathways and rates change. In particular, uraninite and U^{IV}-phosphate oxidize slower because of the formation of a surface layer which inhibits further oxidation. Phosphate also changes the product of uraninite oxidation, which affects the subsequent stability of U^{VI}.

Our recent work also established that U^{IV} is stabilized as mononuclear species by the surfaces of metal oxides. While this finding may explain the observed predominance of mononuclear U^{IV} in field sediments, the contribution of the clay mineral fraction to this effect is unknown. Here, we investigate whether montmorillonite surfaces have a role in the stabilization of mononuclear U^{IV}. An Fe-free clay (SYn-1, 2-100 g/L loading) was reacted with U^{VI} and reducing conditions were established by addition of AH₂DS. Using synchrotron spectroscopy we find that U^{VI} is reduced to nano-particulate uraninite. The predominance of nano-uraninite even at high solids loading suggests that clays do not have as large a role as metal oxides in the stabilization of mononuclear U^{IV}.

An intermediate step in developing field-scale RTMs is testing their predictions in column experiments. The Argonne SFA is using x-ray accessible columns to compare the predicted and measured speciation under advective flow conditions. Results from a column consisting of ferrihydrite-coated packing material and a sulfide-containing influent will be presented.

The Argonne National Laboratory Subsurface Biogeochemical Research Program SFA: Fe and S Biogeochemistry in Redox Dynamic Environments

SBR - ANL SFA (Laboratory Research Manager: Robin Graham)

K. M. Kemner¹ (kemner@anl.gov), D. A. Antonopoulos¹, T. M. Flynn¹, B. Mishra², M. I. Boyanov³, D. E. Latta⁴, M. M. Scherer⁴, C. Liu⁵, J. K. Fredrickson⁵, K. M. Rosso⁵, J. M. Zachara⁵, E. J. O'Loughlin¹

1. Argonne National Laboratory; 2. Illinois Institute of Technology; 3. Bulgarian Academy of Sciences; 4. University of Iowa; 5. Pacific Northwest National Laboratory

Understanding the interplay of the Fe and S biogeochemical cycles with the hydrologic cycle is essential to accurately predict the mobility of contaminants; atmospheric greenhouse gas emissions; carbon cycling and sequestration in subsurface environments; and nutrient mobility in near-surface and subsurface polar, temperate, or tropical systems. The objective of the Argonne Subsurface Biogeochemical Research Program (SBR) Scientific Focus Area (SFA) is *to identify and understand the coupled biotic-abiotic transformations of Fe and S within redox-dynamic environments at the molecular- to core-scale, as well as to understand the effects of Fe and S biogeochemistry on the transformation and mobility of major/minor elements and contaminants.* To accomplish this objective, the Argonne SBR SFA integrates two key analytical strengths at Argonne — the Advanced Photon Source (APS) for synchrotron-based interrogation of systems and next-generation DNA sequencing and bioinformatics approaches for microbial community and metabolic pathway analysis — with biogeochemistry and microbial ecology. Addressing this objective contributes directly to the goal of the United States Department of Energy (DOE), Office of Biological and Environmental Research (BER), Climate and Environmental Sciences Division (CESD) to “advance fundamental understanding of coupled biogeochemical processes in complex subsurface environments to enable system-level environmental prediction and decision support.”

Argonne SBR SFA research addresses four critical knowledge gaps: *(1) an in-depth understanding of the molecular processes affecting Fe, S, and contaminant speciation in dynamic redox environments; (2) an understanding of the role of biogenic and abiotic redox-active products and intermediates in Fe, S, and contaminant transformations; (3) a mechanistic understanding of the factors controlling the mass transfer of Fe, S, and contaminants in heterogeneous media; and (4) an in-depth understanding of the relationship between microbial community dynamics/function and coupled biotic-abiotic controls, and their effects on major/minor element cycling and contaminant transformations.*

The long-term vision of the Argonne SBR SFA envisions ultimately integrating the new mechanistic knowledge generated by the SFA into multiscale Earth system models to enhance their predictive power for relevant environmental processes. The ten year vision also includes (1) an ever-increasing emphasis on integrating metagenomic-based analysis approaches for understanding ecological and functional controls on the biogeochemistry of Fe and S, (2) an increasing emphasis on model development to predict the transformations and mobility of nutrients and contaminants in many subsurface and near-surface environments, and (3) expansion of these studies with a greater emphasis on using minerals and microbial communities from a network of field sites encompassing many types of redox-dynamic environments.

Abiotic redox dynamics between Hg and Mn

SBR - ANL SFA (Laboratory Research Manager: Robin Graham)

Bhoopesh Mishra^{1,2}, Edward J. O'Loughin², Maxim I. Boyanov^{2,3}, Kenneth M. Kemner²

¹Physics, Department, Illinois Institute of Technology, Chicago, IL (USA); ²Biosciences Division, Argonne National Laboratory, Lemont, IL (USA); ³Institute of Chemical Engineering, Bulgarian Academy of Sciences, Sofia, (Bulgaria)

Our studies over the past few years demonstrated that Hg^{II} can be reduced to Hg⁰ by various forms of Fe^{II} due to the comparatively higher redox potential of many Hg^{II}/Hg⁰ couples. Hence we expanded our research and tested the potential for reduction of Hg^{II} by Mn^{II}, as Mn is Earth's second most abundant transition metal next to Fe and is similar to Fe in several aspects of its geochemistry.

Reduction of Hg^{II} by Mn^{II} was tested in batch experiments and solids were characterized by XAFS. Our results show that at pH 7.5, the majority of Hg^{II} is reduced to Hg⁰ within three hours. Hg^{II} reduction is coupled with oxidation of soluble Mn^{II} to highly insoluble Mn^{IV} oxide. Formation of a Mn^{IV} oxide mineral auto-catalyzes the reaction for the first few hours, followed by significantly slower rates of Hg^{II} reduction concomitant with changes in the Mn^{IV} mineral phase. The presence of redox inactive mineral surfaces (e.g. Al₂O₃ and TiO₂) inhibits the rate of Hg^{II} reduction. Hg^{II} reduction by Mn^{II} results in the formation of meta-stable Hg^I species when complexing ions such as sulphate are present, followed by slow transformation to Hg⁰ over an extended period of time.

Under an appropriate change in condition (e.g. pH fluctuation) due to rainfall or storm events, Mn^{IV}-oxides formed as a result of Hg^{II} reduction may become oxidants and re-oxidize Hg⁰, enabling Mn to play a dual role of reductant as well as oxidant of Hg in natural systems. Hence, we also tested the ability of Mn^{IV}-oxides to oxidize Hg⁰ in batch experiments characterizing solids using XAFS. Our results suggest that under acidic pH conditions Mn^{IV}-oxides (e.g. β-MnO₂) can oxidize Hg⁰. Even though oxidation of Hg⁰ by Mn^{IV} is not an unexpected result because Mn^{IV} has been shown to oxidize other contaminants (e.g. Cr^{III} and U^{IV}), the oxidative pathway of Hg⁰ by Mn^{IV} has immense implications on subsurface Hg biogeochemistry in light of recent findings showing biogenic Mn oxide mineral coatings on subsurface geomedia. Clearly, Hg-Mn interactions could have important implications in redox cycling environments due to coupled reduction and subsequent oxidation of Hg by Mn under circumneutral and acidic pH conditions, respectively. Incorporating these newly found Hg redox pathways in global Hg cycle models may improve the prediction of Hg transport, as well as the estimation of the size of the pool of bioavailable Hg for biochemical processes like methylation.

Effects of soluble electron shuttles on microbial Fe(III) reduction and methanogenesis in wetland sediments

SBR - Argonne SFA (Laboratory Research Manager: Robin Graham)

E. O'Loughlin (oloughlin@anl.gov), M. Sladek, D. Antonopoulos, T. Flynn, J. Koval, C. Marshall,
and K. Kemner

Biosciences Division, Argonne National Laboratory

Iron redox cycling by microorganisms is a significant component of C cycling and energy flux in many aquatic and terrestrial environments. Dissimilatory iron-reducing bacteria (DIRB) are phylogenetically diverse microorganisms that obtain energy by coupling oxidation of organic compounds or H₂ to reduction of Fe(III) to Fe(II). Because of the relative insolubility of most Fe(III)-bearing minerals, many DIRB use soluble electron shuttles (e.g., quinones, flavins, phenazines, and reduced sulfur species) to transfer electrons from the cell to external electron acceptors. Studies investigating effects of electron shuttles on microbial Fe(III) reduction have typically been conducted under axenic conditions. To better understand how electron shuttles influences microbial Fe(III) reduction in the presence of a diverse microbial community, we examined the effects of different electron shuttles (9,10-anthraquinone-2,6-disulfonate acid (AQDS), 9,10-anthraquinone-2-carboxylic acid (AQC), and 5-hydroxy-1,4-naphthoquinone (lawsone, NQL)) on the bioreduction of Fe(III) oxide and methanogenesis in microcosms inoculated with wetland sediment. Our results show no significant enhancement of Fe(III) reduction in the presence of NQL or AQC relative to the no shuttle (NS) control; however both the rate and extent of Fe(II) production were enhanced in the presence of AQDS. The onset of methanogenesis was earlier in the presence of AQDS compared to NQL and NS, but in each case methane production was not evident until Fe(II) production plateaued. Methanogenesis was completely inhibited in the presence of AQC, highlighting the potential for electron shuttles to influence microbial processes not involving microbial respiration using insoluble electron acceptors. Systems amended with AQC were dominated by microorganisms classified in the family *Pelobacteraceae* (avg. 45.4% total abundance), while *Geobacteraceae* dominated in microcosms amended with AQDS (30-48%), NQL (51.9%), or NS (37%). *Geobacteraceae* sequences were of much lower abundance in the AQC enrichments, accounting for only 8% of the total abundance on average and only 3–4% in two of the three replicates. While closely related to the *Geobacteraceae*, organisms in *Pelobacteraceae* lack c-type cytochromes and are unable to transfer electrons directly to ferric iron. This suggests AQC may inhibit direct reduction of ferric iron by organisms such as *Geobacter*, allowing *Pelobacter* spp., which would otherwise be outcompeted, to dominate.

LBNL ABSTRACTS

Flood Plain Modeling: Hydrological, Biogeochemical, and Microbial Controls on Carbon and Nitrogen Fluxes

Dipankar Dwivedi, Bhavna Arora, Nicolas Spycher and Carl Steefel

2-D and 3-D reactive flow and transport modeling was used to address the principal controls on carbon and nitrogen cycling in the Rifle and lower East River, Colorado flood plains. The objectives of this work are to: (1) quantify the impact of biogeochemical hot spots (e.g., hyporheic zones, reduced minerals) and hot moments (e.g., river water/ground water fluctuation) on carbon and nutrient fluxes at flood plain/watershed scales, and (2) understand the role of including microbial complexity in reaction networks.

At the Rifle site, the modeling group has led to the development of a 2-D genome-informed reactive-transport model to investigate the impact of localized biogeochemically reduced zones (referred to as naturally reduced zones or NRZs) as well as hot moments on vertical and lateral carbon fluxes. The 2-D model was based on a site-specific reaction network that was informed by genomic studies which explicitly accounted for the previously identified chemolithoautotrophic processes at the site. Importantly, the 2-D modeling efforts suggested that the genome-informed reaction networks and representation of hotspots and hot moment significantly improved prediction of carbon cycling at the Rifle flood plain.

At the lower East River Watershed study site, our efforts have focused on evaluating the importance of hyporheic zone interactions on carbon and nitrogen cycling. Upwelling of nutrient-rich water and downwelling of higher pH and dissolved oxygen rich-water can lead to distinct biogeochemical gradients within the hyporheic zone. To understand the impact of hyporheic exchanges on hydrological and biogeochemical fluxes at the meander scale, we integrated a genome-informed reaction network (similar to the Rifle site model) with a high-resolution, 3-D reactive transport solver - PFLOTRAN. 3-D modeling results demonstrate that the intra-meander hyporheic flow paths and biogeochemical reactions cause the lateral redox zonation, which considerably impact the carbon and nitrogen fluxes into the stream system. Also, the meander-driven hyporheic flow paths enhance denitrification because of relatively longer residence times of nitrate in the organic carbon-rich sediments.

The work also includes the development of scaling constructs based on high resolution 2-D and 3-D reactive transport modeling to capture explicitly the scale-dependence of the hydrological and biogeochemical fluxes across the important subsystem compartment of the floodplain, with inputs from both the upstream river system, adjacent hillslopes, and the deeper shale bedrock compartments.

Using strain-resolved metatranscriptomic analysis to highlight active biogeochemical processes in the subsurface

T. N. M. Jewell¹, U. Karaoz¹, J. F. Banfield², E. L. Brodie¹, K. H. Williams¹, **H. R. Beller¹**

¹ Lawrence Berkeley National Laboratory, ² University of California, Berkeley

Metatranscriptome data represent the *realized* metabolic potential of microbial communities. During the first phase of the Berkeley Lab Subsurface Biogeochemistry Genomes-to-Watershed SFA (SFA 2.0), strain-resolved metatranscriptome data were used to leverage metagenome data to highlight the most active metabolic pathways under conditions of interest at the Rifle (CO) site. Here, we summarize significant and often unexpected metatranscriptomic findings made during two Rifle studies: (1) a nitrate perturbation field experiment that explored subsurface N cycling and (2) a microcosm experiment revealing active metabolic pathways in naturally reduced zones (NRZ), which are biogeochemical hot spots at Rifle. Overall, these data provided key insights into biogeochemical cycling in the Rifle subsurface, including the important role of chemolithoautotrophy, and have been used to inform GEWaSC (Genome-Enabled Watershed Simulation Capability) modeling efforts for SFA 2.0.

In a two-month study of nitrate amendment to the perennially suboxic Rifle aquifer, strain-resolved metatranscriptomic analysis revealed pervasive and diverse chemolithoautotrophic bacterial activity relevant to C, S, N, and Fe cycling (Jewell et al. 2016, *ISME J*). Prior to nitrate injection, anaerobic ammonia-oxidizing (anammox) bacteria accounted for 16% of overall microbial community gene expression, whereas during the nitrate injection, two other groups of chemolithoautotrophic bacteria collectively accounted for 80% of the metatranscriptome: (1) members of the Fe(II)-oxidizing Gallionellaceae family and (2) strains of the S-oxidizing species, *Sulfurimonas denitrificans*. Notably, the proportion of the metatranscriptome accounted for by these three groups was considerably greater than the proportion of the metagenome coverage that they represented. Transcriptional analysis revealed some unexpected metabolic couplings, in particular, putative nitrate-dependent Fe(II) and S oxidation among nominally microaerophilic Gallionellaceae strains, including expression of periplasmic (NapAB) and membrane-bound (NarGHI) nitrate reductases. The three most active groups of chemolithoautotrophic bacteria in this study had overlapping metabolisms that allowed them to occupy different yet related metabolic niches throughout the study.

In a 3-week study of anaerobic microcosms inoculated with Rifle NRZ sediments as the sole source of carbon and microbes, metatranscriptomic data elucidated active metabolic pathways in these biogeochemical hotspots. Successions in biogeochemical activity and microbial community composition were observed throughout the experiment. For example, putative members of the Chloroflexi and chemolithoautotrophic *Sulfuricurvum* taxa were initially active but decreased markedly over time. In contrast, putative members of the *Hydrogenophaga* and *Dechloromonas* genera emerged to be among the most active strains during the study (with one *Hydrogenophaga* strain accounting for up to ~30% of the metatranscriptome). Among the most surprising findings were the following: (1) a relatively small number of bacteria accounted for a substantial proportion of sample metatranscriptomes, (2) active denitrification by *Hydrogenophaga* and *Dechloromonas* strains occurred even though nitrate concentrations were low ($\leq 120 \mu\text{M}$), and (3) the most dominant *Hydrogenophaga* strain catalyzed chemolithoautotrophic activity (S and H₂ oxidation) as well as heterotrophic activity.

Genome-enabled modeling of microbial biogeochemistry using a trait-based approach. Does increasing metabolic complexity increase predictive capabilities?

E. KING¹, S. MOLINS¹, U. KARAOZ¹, N.J. BOUSKILL¹, K. ANANTHARAMAN², H.R. BELLER¹, T. N. M. JEWELL¹, K.H. WILLIAMS¹, J.F. BANFIELD^{1,2}, C.I. STEEFEL¹, S.S. HUBBARD¹, E.L. BRODIE^{1,2*}

¹Lawrence Berkeley National Laboratory, ²University of California, Berkeley

*elbrodie@lbl.gov

The biogeochemical functioning of ecosystems is shaped in part by genomic information stored in the subsurface microbiome. Cultivation-independent approaches allow us to extract this information through reconstruction of thousands of genomes from a microbial population. Analysis of these genomes, in turn, gives an indication of the organisms present and their functional roles. However, metagenomic analyses can currently deliver thousands of different genomes that range in abundance/importance, requiring the identification and assimilation of key physiologies and metabolism to be represented as traits for successful simulation of subsurface processes.

Here we focus on incorporating -omics information into BioCrunch, a genome-informed trait-based model that represents the diversity of microbial functional processes within a reactive transport framework. This approach models the rate of nutrient uptake and the thermodynamics of coupled electron donors and acceptors for a range of microbial metabolisms including heterotrophs and chemolithoautotrophs. Metabolism of exogenous substrates fuels catabolic and anabolic processes, with the proportion of energy used for cellular maintenance, respiration, biomass development, and enzyme production based upon dynamic intracellular and environmental conditions. This internal resource partitioning represents a trade-off against biomass formation and results in microbial population emergence across a fitness landscape.

Biocrunch was used here in simulations that included organisms and metabolic pathways derived from a dataset of ~1200 non-redundant genomes reflecting a microbial community in a floodplain aquifer. Metagenomic data was directly used to parameterize trait values related to growth and to identify trait linkages associated with respiration, fermentation, and key enzymatic functions such as plant polymer degradation. Simulations spanned a range of metabolic complexities and highlight benefits originating from simulations including a larger number of organisms that more appropriately reflect the *in situ* microbial community. Simulations demonstrate the importance of dynamic vs. static energy allocation to predict active processes such as anammox. In addition, even though traditional methods showed no thermodynamic limitations on reaction rates, the maximum potential growth rate of iron reducers were shown to vary spatially by a factor of 2-3 due to differences in energy allocation.

This research is part of the Berkeley Lab Subsurface Biogeochemical Research Genomes-to-Watershed SFA.

Building Observational Networks for Hydrologic Characterization of the Snow-Dominated SFA East River Watershed Study Site

Rosemary W.H. Carroll¹, Lindsay Bearup², Roelof Versteeg³, Greg McCurdy¹, Ben Potter⁴,
Lauren Foster⁵, Reed Maxwell⁵ and Kenneth H. Williams²

Quantifying the timing, intensity and duration of water inputs to snow-dominated watersheds is critical to understanding energy and water budget partitioning with direct consequences on water delivery to streams as well as on hydrologically mediated biogeochemical processes that control nonlinear riverine solute fluxes. Tremendous uncertainty in quantifying boundary condition influxes at the watershed scale is largely due to spatial and temporal heterogeneity in snow-related properties. In addition, scarcity and sampling bias in climate station infrastructure make it difficult to resolve hydrologic variability at scales relevant to biogeochemistry. As part of its Subsurface Biogeochemistry Watershed Function Scientific Focus Area (SFA), Berkeley Lab has recently established the East River (ER) in the mountains of central Colorado. The ER is representative of many high-elevation headwater systems within the Upper Colorado River Basin, with watershed complexity and hard to access terrain compounding difficulties in sampling for adequate understanding of watershed processes. To address these challenges, observation networks related to precipitation and stream fluxes are being developed in concert with a high-resolution, physically-based, integrated hydrologic model and remote sensing/airborne retrieval methods; and will support future work on hydrochemically derived streamflow age distributions. Streamflow is measured at 14 locations using pressure transducers and acoustic Doppler velocimeter (wadable) and current profiler (unwadable) to isolate sub-basin export of water and solutes. Climate monitoring relies on two SNOTEL sites, an EPA CASTNET station and six meteorological stations owned and operated by the Rocky Mountain Biological Laboratory (RMBL). RMBL station upgrades have begun with support from the SFA and the Desert Research Institute, and all climate stations are being incorporated into a sophisticated platform for data retrieval and visualization. Targeted and novel approaches to measure snow water equivalent (SWE) include a verification study of weighing-gage SWE plate technology, with potential for deployment to remote portions of the basin. In addition, comprehensive snow sampling campaigns encapsulate the largest possible range in observed physiographic parameters and will inform future LiDAR surveys being considered by the SFA. Snowmelt isotopic flux is measured at five locations, with a near-instantaneous collection device (Picarro) installed for direct comparison with stream discharge to provide the highest resolution on observed isotopic mass flux. Observation networks are focused on fundamental questions related to water cycling and provide hydrologic characterization for ongoing collaborative projects across scales within the ER watershed.

¹ Desert Research Institute, Reno, NV; rosemary.carroll@dri.edu

² Lawrence Berkeley National Laboratory, Berkeley, CA.

³ Subsurface Insights, Hanover, NH

⁴ Navarro Inc., Grand Junction, CO.

⁵ Colorado School of Mines

Subsurface carbon inventories and fluxes in a semi-arid region floodplain, Rifle Colorado

J. Wan, W. Dong, T. K. Tokunaga, K. H. Williams, Y. Kim, C. Hobson, M. Bill, M. Conrad, P. E. Long, S. S. Hubbard – LBNL

Most understanding on terrestrial carbon cycling is based on investigations of topsoil (typically < 0.3 m, and seldom deeper than 1.0 m), yet about half of the terrestrial organic carbon inventory resides at greater depths. How carbon cycles through the subsurface requires integration of measurements that account for exchanges among atmosphere, vadose zone and groundwater, and eventual exports to rivers. Semi-arid and arid regions account for a large and growing fraction of Earth's surface, where tracking subsurface C fluxes is difficult because of generally lower organic C inventories, low net infiltration, and low rates of groundwater flow. As part of the Berkeley Laboratory's Subsurface Biogeochemistry Genomes-to-Watersheds SFA effort, we are conducting field and laboratory studies on C cycling in a semi-arid floodplain within the Colorado Plateau, at the Rifle, Colorado. Five sampling and monitoring sites were established along a transect aligned with the general direction of groundwater flow, which discharges into the Colorado River at the southern edge of the floodplain. Analyses of soils, vadose zone and aquifer sediments, pore water chemistry, organic carbon (OC) speciation, vadose zone gas composition, soil and sediment respiration rates, combined with measurements of gas and water fluxes provide information needed to quantify inventories and fluxes of inorganic and organic C within the floodplain. These measurements showed that the deeper vadose zone (subrhizosphere) contains total and dissolved organic and inorganic carbon inventories as high as those of the rhizosphere, and DOC levels much higher than in the aquifer. OC is transported to the subrhizosphere from the rhizosphere via spring season infiltration and water table decline following annual recession of the Colorado River's snowmelt dominated stage. Spectroscopic analyses suggest that OC annually transported into the subrhizosphere is relatively bioavailable. Labile OC annual delivery of into the deeper vadose zone is largely metabolized, given moisture, oxygen, and temperature conditions that remain favorable for microbial activity throughout the year. This results in a significant (18%) contribution from the subrhizosphere to the annual floodplain CO₂ flux (~330 g C m⁻² y⁻¹). Very low net infiltration in this semi-arid floodplain combined with elevated respiration rates in the subrhizosphere limit OC transport into groundwater. Relatively low DOC in the aquifer (~0.3 mM) combined with low groundwater velocities (~0.3 m day⁻¹) limit DOC exports from the floodplain into the Colorado River. Thus, vadose zone CO₂ fluxes constitute by far the largest C export from this semi-arid region floodplain.

Chemical Characterization and Release Dynamics of Sediment Associated Organic Matter at the Rifle, Co Field Site

Patricia Fox, Ruth Tinnacher, Xiu Yuan, Jim Davis, Benjamin Gilbert, Peter S. Nico; Lawrence Berkeley National Laboratory, Berkeley, CA, 94720, USA

Patricia Fox, Lawrence Berkeley National Laboratory, Berkeley, CA, United States

Sediment-associated natural organic matter (NOM) is an extremely complex assemblage of organic molecules. The chemical nature of NOM may control its' reactivity towards metals, minerals, enzymes, and bacteria. Total organic carbon (TOC) contents are typically around 0.1% (posing a distinct challenge for characterization), but can range from 0.03% up to approximately 1.5%. Even at the typical TOC values of 0.1%, the mass of sediment-associated OC is approximately 5000 times higher than the mass of dissolved OC (assuming typical DOC values of 1-3mg/l). The goals of this study were two-fold: first, to understand how the chemistry of sediment associated organic matter varied with location across the site, depth relative to water table, and different functionally defined reactive fractions; second, to understand the capacity for mineral associated organic matter to buffer DOC concentrations under varying chemical conditions.

We have characterized sediment-bound NOM from two locations. One location has relatively low organic carbon (<0.2%) and is suboxic [dissolved oxygen is low or absent, but no dissolved Fe(II) observed], while the other is a naturally reducing zone with higher organic carbon (0.2-1.5%) and Fe(II)-reducing conditions. Different NOM fractions [water soluble (MQ-SPE), pyrophosphate–acid soluble (PP-SPE), and pyrophosphate–acid insoluble (PP >1kD)] were extracted and isolated from the sediments and analyzed by a variety of techniques, including UV-Vis, FTIR, and ICP-MS. Each NOM fraction was chemically distinct, with the MQ-SPE and PP-SPE fractions being relatively more similar and distinct from the PP >1kD fraction. The MQ-SPE fraction appears to be more aliphatic and the PP fractions more aromatic as evidenced by both FTIR and UV-Vis data. The MQ-SPE fractions varied more widely across samples than the other fractions, indicating that this represents a much more dynamic pool of sediment-associated NOM.

To understand the DOC buffering capacity of the sediment associated organic matter, aquifer sediments were brought into contact with fresh, organic-carbon free groundwater solutions, at natural or reduced CO₂ concentration levels, in lab-scale batch experiments. During the repeated exchange of solutions at two temperature settings (room-temperature and 4 °C), solution pH and metal and organic carbon concentrations were monitored. Preliminary results for 20 exchanges of groundwater solutions over 50 days, showed an ongoing ability of the sediment associated organic matter to buffer DOC concentrations ~0.4-1mg/L through repeated release of low concentrations of organic carbon (~0.5-2 mg C/g sediment; ~0.05-0.2% of sediment-associated organic carbon) without any apparent depletion in the overall source term during the experiment.

Climate change and land use are significantly reshaping interactions among vegetation, soils, subsurface and fluvial compartments of watersheds throughout the world. While watersheds are recognized as Earth's key functional unit for assessing and managing water resources, hydrological processes in watersheds mediate most, if not all, biogeochemical processes that support terrestrial life. Despite the importance of watershed function to agriculture, energy, urban and other societally important systems, the scientific community is at a preliminary stage of developing a predictive understanding of how watersheds function from a hydrological and biogeochemical perspective, and how they will respond to increasingly frequent perturbations, such as floods and droughts.

The Genomes-to-Watersheds SFA (FY14-FY16) undertook what may have been the first coordinated attempt to gain a predictive understanding of metabolic potential of a terrestrial environment in the context of system-wide fluxes and a range of heterogeneity. Working within the Rifle floodplain of the Colorado River, our experimental and observational efforts transformed what we now know about the subsurface microbiome and their metabolic potential for mediating a wide range of biogeochemical cycles. We documented the role of the vadose zone in carbon cycling at the site, and used geophysical approaches to quantify hot spots in the floodplain that influenced biogeochemical cycling. We developed the first ever genome-enabled biogeochemical watershed simulation capability (GEWaSC), challenged it with diverse field data, and successfully documented the improvement in predictions of biogeochemical cycles and exports to the Colorado River enabled by inclusion of genomic information.

We are now building upon our genome-enabled floodplain advances to predict watershed function and dynamics. In this move to greater scales and complexity, we take a 'system-of-systems' view of the watershed. Recognizing that while it is typically impossible to perform explicit characterization and modeling of a watershed everywhere at high resolution (in the manner previously performed at Rifle, CO), we adopt a scale-adaptive construct that assumes that the integrated watershed response to disturbances (such as floods, droughts and earlier snowmelt) can be adequately predicted through consideration of a limited number of subsystems within the greater watershed system, where the collection of chosen subsystems are assumed to exhibit a range of residence times and reaction rates relevant to water, nutrient, carbon and metals processing within the watershed.

The Watershed Function SFA (FY17-FY19) proposes to develop and test the ability of scale-adaptive approaches to address an **overarching science question of 'how will mountainous watersheds retain and release water, nutrients, carbon and metals downgradient?'** In particular, the SFA will **quantify how warming, early snowmelt and hydrological perturbations will influence mountainous watershed dynamics that impact downstream water availability and biogeochemical cycling at seasonal to decadal timescales.** We propose to initiate this project in a headwater catchment of the Upper Colorado River Basin, perhaps the most important basin in the Western U.S., which supplies municipal water to more than 1 in 10 Americans, irrigation water and nutrients to more than 5.5 million acres of land, and supports more than 4,200 megawatts of electrical generating capacity, and supports diverse ecosystems that provide other societally relevant services. Four theme-based hypotheses have been identified to address the SFA question of how mountainous watersheds retain and release water, nutrients, carbon, and metals downgradient:

- **Hydrology:** Decreased snow cover and earlier snow melt due to warming of mountainous watersheds will reduce overland flow and increase early season infiltration, leading to deeper transport of solutes and increased production of CO₂ within the vadose zone
- **Ecohydrology:** Feedbacks between hydrology-driven changes in vegetation and vegetation-driven changes in hydrology will increase evaporative loss and decouple microbially-mediated biogeochemical processes that control nutrient fluxes in mountainous watersheds
- **OrganoMineral Dynamics:** The intensity of hydrological pulses to floodplain sediments and the hydrologic residence time within shale materials will control the release of carbon, nitrogen, and metals to riverine systems
- **Watershed Reactor:** Hydrologic perturbations to mountainous watersheds lead to nonlinear riverine fluxes of water, carbon, nutrients and metals, which can be predicted using a scale-adaptive framework that takes into account variable residence time versus reactivity relationships associated with subsystems.

This poster will highlight advances made during the past year as part of the Genomes-to-Watershed SFA, and will describe recent research to develop the next Watershed Function SFA and associated scale-adaptive approaches.

Variability in microbial community structure and function across and among meanders in the East River SFA Watershed Study Site

Paula B. Matheus Carnevali¹, Kenneth H. Williams², Karthik Anantharaman¹, Alexander Thomas³, Susan Hubbard² and **Jillian F. Banfield**^{1,2,3}

¹Department of Earth and Planetary Sciences, University of California, Berkeley

²Lawrence Berkeley National Laboratory

³Department of Environmental Science, Policy and Management, University of California, Berkeley (jbanfield@berkeley.edu)

SBR Program - Genomes to Watershed SFA (PI: Susan Hubbard, LBNL)

Microbially-mediated biogeochemical processes that occur at the micron-scale impact watershed function and ecosystem outputs at the tens of kilometers scale. Building from research at the Rifle site on subsurface biogeochemical processes over meter length scales, the new Berkeley Lab Subsurface Biogeochemistry Watershed Function SFA will be conducted at a headwaters catchment (East River) and aims to develop understanding of biogeochemical processes at the watershed scale. Watershed functioning relies on complex interactions among vegetation, hydrology, topography, and geology that lead to distinct environmental compartments at the surface and in the subsurface. We hypothesize that detailed analysis of meanders, important riparian zone compartments, can generate insights about key biogeochemical processes that can be used to approximate the function of the larger system. The meanders were subdivided into river channel, hyporheic zone, and the surface and subsurface vegetated soils and sediments, whose characteristics reflect past and present river flow dynamics. We sampled soils and sediments of meanders close to the headwaters, downstream, and close to the end of the modeling domain of the East River. Our objectives are to infer processes that contribute to C and N cycling based on the metabolic potential of the microbial communities and to identify hotspots and hot moments of microbial activity in the riparian zone and their impacts on nutrients cycling in the watershed. The sampling targeted soil depths ~ 10-25 cm across a grid of sites covering up to 100 m² of terrain over each meander. Ninety-six samples have been submitted to the Joint Genome Institute for metagenomic sequencing. We expect to assemble draft genomes for organisms that represent $\geq 1\%$ of the community. This work will leverage the genome-resolved metagenomic bioinformatics methods developed through research at the Rifle site. This pilot study will allow us to compare the characteristics of the three meanders and to identify patterns of variation of microbial community structure and function, correlated with solid phase geochemical and mineralogical analysis. The research will provide insight into the role of meanders for the overall functioning of the watershed. Although there are likely to be differences in nutrient degradation and other processes among the three different meander sites, we expect to find meaningful commonalities that will support the use of meanders as representative scaling motifs.

Exploring climate controls on hyporheic zone dynamics and feedbacks between sediment distribution, riverbed bioclogging, infiltration, and microbial CO₂ production

Michelle E. Newcomer¹, Susan S. Hubbard², Craig Ulrich², Baptiste Dafflon², John Peterson², Yoram Rubin¹

¹University of California, Berkeley

²Lawrence Berkeley National Laboratory

In regions worldwide, losing rivers are common and can introduce feedbacks affecting total transport of infiltration and nutrients. Permeability decline from hyporheic zone bioclogging is one feedback that is thought to depend on climatic events that control riverbed parameters, primary productivity, and subsurface gas production. River life-cycles are an important component of this cycle as they typically represent a sink of CO₂ gas from the atmosphere. When benthic organisms decay, however, this provides a source of dissolved organic carbon (DOC) to subsurface microbes for transformation back to CO₂. Net CO₂ and other greenhouse gas (GHG) fluxes from the surface-subsurface interface are highly dependent on hyporheic flows, infiltration rates, and groundwater-surface water interactions to facilitate their transformations. Both surface and subsurface metabolism, leading to bioclogging of subsurface sediments are linked to GHG fluxes and are not well quantified in river-aquifer zones. Nor are their interactions and dependencies understood in rivers that have variable surface-water flow and infiltration regimes from climate perturbations such as from the El Niño Southern Oscillation (ENSO).

To address the effect of large scale climate-controls on biogeochemical fluxes, we simulated riverbed biological growth and hyporheic zone carbon dynamics using 1D/2D numerical models, allowing a range of initial grain size distributions (GSD) to represent ENSO control of riverbed scour. GHG fluxes from subsurface microbes were quantified as a function of surface ecological DOC production and river discharge. We modeled primary productivity and DOC production using surface water quality data and samples of phytoplankton from a floodplain located in the upper East River watershed in Colorado (Field site of the LBNL-SBR Subsurface Biogeochemistry Watershed Function SFA). Two model types were considered: 1) river scale river-aquifer flow model, and 2) hyporheic flow model. Within the numerical model, simulated hyporheic flow paths, transformation of DOC to GHGs, and redox conditions allowed precipitation of metals (Fe II and Fe III), and redox-stratified microbial communities that feedback into surface ecological growth.

Our work links climatic perturbations of surface water discharge as a major control on riverbed sediment GSD, bioclogging, and subsurface transformations. Results show that GHG production is not only a function of surface ecology, but linked to the statistics of extreme climatic events that control riverbed initial conditions. These results provide a new understanding of nutrient cycling and hotspot bioclogging in losing rivers where climatic extremes occur.

Deep vadose zone respiration contributions to CO₂ fluxes from a semi-arid floodplain

Tetsu K. Tokunaga, Yongman Kim, Mark E. Conrad, Markus Bill, Chad Hobson, Kenneth H. Williams, Wenming Dong, Jiamin Wan, Mark J. Robbins, Philip E. Long, Boris Faybishenko, John N. Christensen, Susan S. Hubbard

Earth and Environmental Sciences Area, Lawrence Berkeley National Laboratory, Berkeley, CA 94720 USA

Abstract

Although CO₂ fluxes from soils are often assumed to originate within shallow soil horizons (< 1 m depth), relatively little is known about respiration rates at greater depths. As part of the Berkeley Laboratory's Subsurface Biogeochemistry Genomes-to-Watersheds SFA effort, we compared measured and calculated CO₂ fluxes at the Rifle floodplain along the Colorado River, and measured CO₂ production rates of floodplain sediments in order to determine the relative importance of deeper vadose zone respiration. Measurements of soil surface CO₂ fluxes and depth profiles of vadose zone CO₂ concentrations were obtained at five monitoring sites on the floodplain. Calculations based on measured CO₂ gradients and estimated effective diffusion coefficients yielded fluxes that are generally consistent with measurements obtained at the soil surface (330 g C m⁻² yr⁻¹). CO₂ production from the 2.0 to 3.5 m depth interval was calculated to contribute 17% of the total floodplain respiration, with rates that were larger than some parts of the shallower vadose zone and underlying aquifer. Respiration rates determined from laboratory incubations of sediments, and from 2.0 m deep non-isothermal sediment columns are consistent with the field-based measurements. The deeper unsaturated zone typically maintains intermediate water and air saturations, lacks extreme temperatures and salinities, and is annually resupplied with organic carbon from snowmelt-driven recharge and by water table decline. These conditions support deeper unsaturated zone respiration throughout the year, and influence vadose zone-aquifer interactions.

Agile data management and synthesis for heterogeneous, multiscale watershed datasets

Charuleka Varadharajan, Boris Faybishenko, Roelof Versteeg and Deb Agarwal

The goal of the data management and assimilation (DMA) component of the U.S. DOE's Genomes to Watershed and Watershed Function Science Focus Areas (SFA) is support of SFA data management needs and efficient generation of data synthesis products to enable SFA science and render datasets available for community use. The objective is to create a software platform to enable users to integrate diverse and disparate field, laboratory, and simulation datasets, including geological, geochemical, geophysical, microbiological, hydrological, and meteorological data across a range of spatial and temporal scales within the Rifle floodplain and the East River watershed, Colorado.

Development priorities of data products are dynamically driven by project science needs. Agile development and modified User-Centered Design (UCD) techniques have and will continue to be used to develop synthesis products, and common infrastructure to archive SFA-generated data, obtain external datasets, perform quality assurance and quality control (QA/QC), perform gap-filling, implement synthesis pipelines, provide user analytics interfaces, support parameter estimation, implement uncertainty quantification, and manage data.

In the Genomes to Watershed SFA, data collection and QA/QC activities have focused on data and products needed for on-going scientific analyses, and hydrological and geochemical modeling. Sensor-based datasets from the DOE-LM installed System Operation and Analysis at Remote Sites (SOARS) network that collects data from water-level pressure transducers, vadose zone and groundwater thermistors, and meteorological stations, as well as data from laboratory characterization of groundwater samples have been curated and archived in a database. An example of an accomplishment is development of automated QA/QC methods to identify and flag issues in the data. Based on the analysis of field water-level data, we provided recommendations on reinstallation and calibration of pressure transducers installed in monitoring wells. Additionally, in support of QC of the geochemical dataset, we developed an approach of flagging samples based on an evaluation of the ionic balance of water samples. Additionally, we have developed, tested and released a broker and portal that integrates the diverse datasets from the different distributed databases where project data are curated. The development of the portal user interface followed UCD methods, resulting in an intuitive product that presents the highest priority datasets and capabilities needed by users including data search, visualization and download.

Our agile approach has enabled us to build a DMA system that is keeping pace with the project science needs while utilizing limited resources.

Above and Below-Ground Geophysical Characterization of Watershed Structure and Functioning

H.M. Wainwright¹, B. Dafflon¹, Y. Wu¹, A.P. Tran¹, K.H. Williams¹ and S.S. Hubbard¹
¹Lawrence Berkeley National Laboratory

Predictive understanding of watershed function and dynamics is hindered by lack of means to quantify complex interactions between plants, minerals, microbes, dissolved constituents, and migrating fluids. These multi-scale interactions and feedbacks occur from bedrock-to-canopy, and variably within the watershed as a function of landscape position and environmental gradients. A key aspect of the Berkeley Lab Subsurface Biogeochemistry SFA is to develop new characterization and monitoring methodologies to quantify complex watershed systems, using new sensing, inversion, and data assimilation approaches. In particular, we aim to (a) tractably identify the regions that have unique suites of properties that influence watershed subsystem behavior (b) provide unparalleled insights about the interactions between above and below-ground processes and their responses to disturbances; (c) provide unprecedented understanding of in-situ fine-scale processes, such as microbially-mediated root zone functions and dynamics. We have developed and tested several approaches at the Genomes-to-Watershed Rifle CO site, and are extending and expanding our methods to the new East River SFA Watershed Study Site. Examples include:

- In situ electrical resistance tomography (ERT) imaging to investigate root-zone dynamics, including: (1) identifying important plant root traits and their adaptation to environmental conditions, (2) tracking root zone water and nutrient dynamics regulated by hydraulic redistribution and (3) understanding how below ground root trait dynamics impact above ground plant growth and productivity.
- A new autonomous sensing methodology to jointly collect subsurface measurements (using ERT and point sensors) and land surface measurements (sensors mounted on poles and unmanned aerial system) to, for the first time, 'watch' bedrock-through-canopy interactions, particularly in response to perturbations.
- New inversion approaches that can incorporate streaming field data to estimate the spatiotemporal dynamics of subsurface properties important for microbial activity, such as heat, water and nutrient fluxes. The new inversion framework has been tested at the Rifle, CO site with autonomously collected above-and-below ground datasets to explore responses to snowmelt and infiltration/evaporation processes.
- Statistical approaches to quantify hot spots and functional zones in the landscape, using multi-scale datasets. The zonation approach provides a tractable approach to capture co-variability among various subsurface and surface properties (such as plant functional types and dynamics, geomorphology, soil thickness and soil biogeochemical properties), and to distribute those properties for parameterizing watershed-scale ecosystem models.

These and other Watershed Function SFA geophysical activities are leading to the development of a 'Digital Watershed'.

From Rifle to RMBL: MODEX activities at Berkeley Lab's East River Watershed Study Site

KENNETH H. WILLIAMS¹, ROSEMARY CARROLL², WENDY BROWN³, CHAD HOBSON¹, REED MAXWELL⁴, SUSAN S. HUBBARD¹

¹*Lawrence Berkeley National Laboratory*, ²*Desert Research Institute*, ³*Bugs Unlimited, LLC*, ⁴*Colorado School of Mines*

As part of its Subsurface Biogeochemistry Watershed Function Scientific Focus Area (SFA), Berkeley Lab and its collaborating institutions have initiated Modeling-Experiment (MODEX) activities within the upper East River watershed designed to assess the impact of climate disturbance on the retention and release of water, nutrients, carbon, and metals from mountainous systems. The East River SFA Watershed Study Site encompasses the drainages of the East River, Washington Gulch, Slate River, and Coal Creek. The 300km² watershed is located northeast of Crested Butte, CO at an average elevation of 3266m. Spanning 1420m of topographic relief, pronounced gradients exist in hydrology, geomorphology, biome type (montane, subalpine, alpine), and extent of impact by mining and mineralized rock, with Slate River and Coal Creek more heavily impacted by heavy metals than the East River and Washington Gulch drainages. The watershed receives an average of 980mm of precipitation per year, the bulk of which falls as snow, and is representative of many headwaters systems within the upper Colorado River Basin. The more 'pristine' East River drainage covers an area of 180km² and is home to the Rocky Mountain Biological Laboratory (RMBL), which provides an extensive experimental and observational database critical to quantifying ecohydrological functioning within the watershed. RMBL facilitates data generation and sharing related to meteorology, phenology, experimental warming, plant water utilization, and coupled vegetation-microbiology studies of direct relevance to the SFA and its DOE-funded partners.

Excursions in stream water discharge are driven primarily by snowmelt, with summer/fall rainfall inducing punctuated increases in flow. Hydrogeochemical data indicate strong variations in water isotope composition of stream waters within the catchment as a function of time suggesting distinct and seasonally dependent reservoirs contributing to flow. Initial observations suggest varying responses in nutrient concentration to stream flow, with nitrate and sulfate generally positively and inversely correlated with discharge. Primary export of dissolved organic carbon accompanies the annual spring freshet, with episodic release accompanying discrete summer/fall rain events. Hyporheic exchange between the East River and its floodplain deposits induces sharp gradients in redox active elements, such as iron, sulfur, and carbon, with gaining reaches exhibiting evidence of reducing conditions resulting from processing of solid and aqueous phase constituents.

The catchment is being modeled at 10m resolution using ParFlow, a parallel, integrated hydrologic model. Driven by meteorological forcing, ParFlow is able to capture land surface processes and represents surface and subsurface interactions through saturated and variably saturated heterogeneous flow.

Rifle Floodplain Water Table Dynamics: Biogeochemical Cycling and Uranium Mobility

S Yabusaki¹, M Wilkins², Y Fang¹, K Williams³, B Arora³, J Bargar⁴, H Beller³, N Bouskill³, E Brodie³, J Christensen³, M Conrad³, R Danczak², E King³, N Spycher³, C Steefel³, T Tokunaga³, R Versteeg⁵, S Waichler¹, H Wainwright³

¹Pacific Northwest National Laboratory, ²Ohio State University, ³Lawrence Berkeley National Laboratory, ⁴Stanford Synchrotron Radiation Lightsource, ⁵Subsurface Insights

Coupled-process modeling is used to build a systematic understanding of the interplay of hydrology, geochemistry, and biology controlling the cycling of carbon, nitrogen, oxygen, iron, sulfur, and uranium in a shallow aquifer-vadose zone-river hydrologic system situated in a floodplain of the Colorado River in Rifle, Colorado, USA and the site of Berkeley Lab's Subsurface Biogeochemistry Genomes-to-Watershed SFA. For most of the year, the floodplain aquifer is generally deficient in oxygen and nitrate. During the snowmelt-driven water table rise and fall in early summer, oxygen and nitrate in the previously unsaturated vadose zone is mixed into groundwater near the water table. The temporal and spatial variation of the biogeochemical response to this event provides an opportunity to characterize process and property interactions responsible for observed behaviors. Some of these behaviors can be linked to distinct zones that reflect the prehistory of the site, including the preferential deposition of organic material and, more recently, the management of uranium mill tailings. Naturally reduced zones have sediments higher in organic carbon and iron sulfides that are linked to faster oxygen consumption, more sulfate and nitrate reduction, and chemolithoautotrophy. Three-dimensional variably-saturated flow and multicomponent biogeochemical reactive transport modeling is used as a systematic framework for interpreting the impact of different material zones, processes responsible for maintaining anoxic conditions, the response to the seasonal water table peaking event, and the redox cycling required to sustain the seasonal behaviors. The biological modeling includes functional representation of fermenters, aerobes, nitrate reducers, sulfate reducers, and chemolithoautotrophs (e.g., microorganisms catalyzing the oxidation of reduced iron, sulfur, and nitrogen). The modeling results are consistent with the oxidation and mobilization of iron, sulfur, and uranium in the background aquifer and NRZs. The mobilization of uranium during the seasonal water table peak is consistent with the oxidation of monomeric U(IV) by biogenic nitrite, and the leaching of surface-complexed U(VI) in the vadose zone. Omics and isotope fractionation have been particularly useful in conceptualizing processes where the absence of measurable concentrations of rapidly-consumed substrates can be problematic.

LLNL ABSTRACTS

The objective of the LLNL SFA Thrust 1 is the further development of a mechanistic understanding of the dominant processes controlling actinide migration in the environment. The research is primarily focused on plutonium. However, we have expanded some of the research to include Np so as to exploit the similarities and differences between these actinides and develop a deeper understanding of their behavior in the environment.

The overarching hypothesis for Thrust 1 is:

***Hypothesis:** The biogeochemical mechanisms controlling **redox transformations of actinides and their stabilization** as aqueous complexes, binary surface complexes, ternary surface complexes, precipitates, and co-precipitates will determine actinide migration in the environment.*

In order to test our hypothesis, we have divided this thrust into the following 6 focus areas:

- A. *Identifying the Mechanisms Driving Surface-Mediated Reduction of Pu and Np*
- B. *The Effect of Natural Organic Matter on Pu and Np Redox Transformations and Sorption Reactions*
- C. *Characterizing the Structural and Chemical Behavior of Pu Nanocolloids*
- D. *Probing the Role of Microbes in Manipulating Pu Behavior*
- E. *Simulating the Molecular-Level Behavior of f-Elements*
- F. *Characterizing Molecular Level Actinide Complexes and Redox Transformations*

In this presentation, we examine how natural organic matter affects the sorption behavior and reduction of Pu(V). First, we describe the role of extracellular polymeric substances in the reduction of Pu(V), the subsequent sorption of Pu as Pu(IV), and the inhibition of Pu(IV) intrinsic colloid formation as a result of Pu-EPS complexation. Second, the role of hydroxamate functional groups, prevalent in siderophore compounds, as reducing agents as well as Pu complexants is explored through a combination of UV-Vis spectroscopy and GC-MS characterization of hydroxamate hydrolysis rates and hydrolysis products. These experiments represent the start of a comprehensive investigation into the natural organic matter functional groups that control Pu redox transformations and complexation in the environment.

The objective of LLNL's SFA is to *identify and quantify the biogeochemical processes that control the fate and transport of actinides in the environment*. The research approach of our Science Plan is to combine (1) **Fundamental Mechanistic Studies** that identify and quantify biogeochemical processes that control actinide behavior in solution and on solids, (2) **Field Integration Studies** that investigate the transport characteristics of Pu and test our conceptual understanding of actinide transport, and (3) **Actinide Research Capabilities** that allow us to achieve the objectives of this SFA and provide new opportunities for advancing actinide environmental chemistry.

Research Thrusts 1 and 2 are guided by broad central hypotheses:

*Thrust 1 Hypothesis: The biogeochemical mechanisms controlling **redox transformations of actinides and their stabilization** as aqueous complexes, binary surface complexes, ternary surface complexes, precipitates, and co-precipitates will determine actinide migration in the environment.*

*Thrust 2 Hypothesis: The biogeochemical processes that ultimately control actinide subsurface mobility/immobility are driven by local variations in the geology, geochemical conditions, colloid composition and abundance, and **chemical characteristics of the initial actinide source**.*

Research Thrust 3 is not hypothesis driven. Instead, it is guided by the research efforts and capability development needs described in Research Thrusts 1 and 2.

Detailed descriptions of the Research Thrusts and associated Focus Areas will be presented in the poster. The new structure of our LLNL's SFA Science Plan reflects the research progress that we have made since the FY12 SFA review and an increased focus on Field Studies and Actinide Research Capabilities that we have chosen to implement in this Science Plan. Since its inception in FY10, our SFA research has made significant progress in identifying the mechanistic processes governing Pu sorption, desorption, complexation, redox transformations, precipitation, and the associated rates of reaction. While our mechanistic understanding of processes controlling Pu transport is far from complete, there is a compelling need to begin evaluating our conceptual and mechanistic understanding from the perspective of remediation and long-term stewardship of legacy sites. This is the focus of Research Thrust 2. The development of new Actinide Research Capabilities stems from our substantial investment in applying unique spectroscopic and numerical approaches to actinide environmental chemistry. These capabilities have led to a number of collaborations with the broader international actinide environmental science community. The intent is to develop these capabilities to achieve the scientific objectives of our SFA and provide unique research capabilities to the broader scientific community.

Our SFA is focused on improving our conceptual understanding of actinide transport in the environment by integrating molecular-scale and field scale observations. The intended goal is to provide the scientific basis for remediation and long-term stewardship of DOE's legacy sites and, more broadly, increase our understanding of and enable predictive control of phenomena in environmental systems sciences.

The success of our program relies on the development and use of state-of-the-art spectroscopic and computational capabilities that are unique to LLNL. Development of these spectroscopic and computational capabilities is intended to benefit the scientific community as a whole. Our intent is for our SFA to be a hub for world-class, U.S. and international radiochemistry research and education. The LLNL SFA has already led to a number of synergistic activities that take advantage of LLNL's unique capabilities and staff. They include i) the development of ultra-trace Np measurements to resolve NNSA-EM contamination questions at the NNSS (formerly NTS), ii) applying NMR and TEM capabilities to actinide separations (collaboration with the former H. Nitsche group), iii) applying Pu TEM capabilities to Nuclear Energy, Used Fuel Disposition, iv) development of NanoSIMS techniques for actinide detection at nanometer spatial scales and sub ppm levels of contamination, v) unprecedented femtomolar detection of Pu using the accelerator mass spectrometry facility at CAMS, and vi) providing LLNL's unique capabilities to visiting students and collaborators.

Research Thrust 3 of the LLNL SFA is focused on the development of state-of-the-art actinide research capabilities that are essential to the success of our SFA Science Program and provide new opportunities for the broader actinide and environmental systems science communities. We have highlighted five capabilities:

- A. *NMR and EPR of Actinide Complexes*
- B. *NanoSIMS of Actinides*
- C. *Actinide TEM-EELS*
- D. *Actinide Analysis at the Center for Accelerator Mass Spectrometry (CAMS)*
- E. *f-Element Ab Initio Modeling*

In this presentation, we will highlight the progress made to date in Ab Initio modeling of Pu hydrolysis and water coordination for $\text{Pu}(\text{OH})_x$ ($x=1-4$) and development of Auxiliary Field Quantum Monte Carlo (AFQMC) for the accurate calculation of redox potentials of aqueous actinide ions. In addition, we describe recent efforts to examine ligand exchange rates and mechanisms for a number of Np(VI) species.

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ORNL ABSTRACTS

Periphyton biofilms generate methylmercury in a contaminated creek system

Todd A. Olsen (olsenta@ornl.gov), Andrew J. King (kingaj@ornl.gov), and Scott C. Brooks (brookssc@ornl.gov)

Environmental Science Division, Oak Ridge National Laboratory, Oak Ridge, TN

Subsurface Biogeochemical Research Program: ORNL Mercury SFA (PI: E.M. Pierce)

Previous SFA research on mercury methylation in East Fork Poplar Creek (EFPC) in Tennessee implies key controls on net methylation occur within the stream or on the stream bed. The large diel variability in dissolved methyl mercury (MeHg) concentration appears to be correlated with the daily photocycle and the sparse wetlands (< 3% watershed area) are poorly connected to the main channel of the creek. Mercury methylation is mediated by bacteria and archaea under anaerobic conditions (Fe(III) or SO_4^{2-} reducing, fermentative, methanogenic). Methylmercury is generated in anaerobic zones within fine-grained channel margin deposits along the creek but the limited extent of these deposits, coupled with the low rates of Hg methylation, suggest these locations account for only a portion of the MeHg in the water.

This phase of our research is designed to elucidate the role of periphyton biofilms in MeHg production in the creek. Periphyton biofilms are complex assemblages of bacteria, fungi, algae, diatoms, invertebrates, detritus, mineral particles and extracellular polymers that grow on submerged surfaces in most aquatic systems. Periphyton is ubiquitous throughout the creek and redox gradients created by microbial metabolism within them support Hg-methylating microbial activity even though the bulk water is well oxygenated (mean DO = 9 mg l⁻¹). Periphyton growth surfaces deployed at upstream (closer to the historic point source of contamination) and downstream locations (~17 km apart) are collected following ~12 weeks colonization in the creek. These samples are subsequently used in laboratory assays of inorganic Hg methylation and MeHg demethylation. Enriched stable isotopes of the Hg species are employed to distinguish new activity from ambient background levels during incubations. In collaboration with Task 3 of the SFA subsamples for microbial community analysis and *hgcAB* gene abundance and phylogeny are also collected. Redox gradients within the periphyton samples are quantified using voltammetric microelectrodes.

Results to date demonstrate that both mercury methylation and MeHg demethylation occur within the periphyton biofilms. Microelectrode profiling shows steep redox gradients within these thin biofilms transitioning from microaerophilic at the biofilm-water contact to sulfate reducing conditions over a distance of 1.5 mm. Although both methylation and demethylation occur in the periphyton, the rate of methylation is greater than the rate of MeHg demethylation indicating periphyton is a net source of MeHg to the creek. Clear differences in methylation and demethylation activity exist between the upstream and downstream sites and across seasons. Samples from the downstream site support higher rates of net MeHg production, consistent with our long-term data record demonstrating increasing MeHg concentration with downstream distance. The differences in net methylation are driven by decreasing demethylation rate constants along the creek as methylation rate constants are comparable between sites. Similarly, all the three major clades of microbial methylators are present at the downstream site

(methanogenic archaea, sulfate reducing firmicutes, and sulfate reducing delta-proteobacteria). These data suggest the downstream periphyton is more complex and contains a greater diversity of redox conditions in comparison to the upstream site, which is dominated by sulfate reducing firmicutes.

Early experimental evidence indicates important environmental conditions that exert control on net MeHg production. Pseudo-first-order rate constants for methylation decrease $\sim 2\times$ with a 10°C decrease in temperature whereas the rate constants for demethylation did not change with temperature. Samples grown in the light but incubated in the dark and samples grown in the dark and incubated in the dark have substantially lower methylation rates suggesting a direct link between active photosynthesis in the periphyton supporting Hg methylation activity by microbes within the biofilm. Ongoing efforts seek to further understand the mechanisms underlying these connections.

High-Resolution Mass Spectrometric Analyses of Mercury-DOM Complexation and Cellular Response of *Geobacter sulfurreducens* PCA Following its *hgcAB* Gene Deletion

Hongmei Chen, Benjamin Mann, Chen Qian, Alexander Johs, Xia Lu, Liyuan Liang, Eric Pierce,
Robert Hettich, Baohua Gu

Oak Ridge National Laboratory, Oak Ridge, TN 37831

Subsurface Biogeochemical Research Program: ORNL Mercury SFA (PI: E.M. Pierce)

Contact: Hongmei Chen (Chenh2@ornl.gov) or Baohua Gu (Gub1@ornl.gov)

Naturally dissolved organic matter (DOM) forms strong complexes with mercury (Hg), affecting Hg chemical speciation, transformation, and bioavailability in aquatic environments. However, exact DOM molecular compounds that react with Hg remain unclear because of the heterogeneous nature and complex composition of DOM. We applied Fourier transform ion cyclotron resonance mass spectrometry coupled with electrospray ionization (ESI-FTICR-MS) to directly probe the formation of Hg-DOM complexes and compositional changes of DOM following its interactions with Hg. Hg-containing DOM molecules were directly identified, with their molecular formulae confirmed by corresponding Hg isotopic peaks present in the mass spectra. A common moiety of $-N_2S_4$ was found in most of the identified Hg-containing DOM formulae, indicating high affinity interactions between Hg and S- and N-containing functional groups in DOM. Most of the “lost” and “new” DOM molecular formulae after reaction with Hg were found to contain S, N, and O, consistent with the view that Hg(II) forms strong complexes through a two-fold coordination involving one reduced S and one O or N in DOM.

Meanwhile, mass spectrometric shotgun proteomics was used to identify differences in the proteome expression between wild-type *Geobacter sulfurreducens* PCA and a $\Delta hgcAB$ mutant, which is deficient in Hg-methylation genes, *hgcA* and *hgcB*, and between wild type and a $\Delta omcBESTZ$ mutant, which is deficient in five outer-membrane *c*-type cytochromes OmcB, OmcE, OmcS, OmcT, OmcZ, required for dissimilatory metal reduction. We were able to delineate the global response of *G. sulfurreducens* PCA in both mutants and identify cellular networks and metabolic pathways that were affected by the loss of these genes. Deletion of *hgcAB* increased the expression of most *c*-type cytochromes, consistent with our previously observed increase in Hg reduction in the $\Delta hgcAB$ mutant. Deletion of *omcBESTZ* was found to increase expression levels of various methyltransferases, indicating that a loss of dissimilatory reduction capacity resulted in elevated activity among one-carbon metabolic pathways. This result also agrees with experimentally determined high rates of Hg methylation by the $\Delta omcBESTZ$ mutant. Additionally, enzymes associated with the folate branch were found to be under-represented in the $\Delta hgcAB$ mutant strain relative to the wild type, which supports the hypothesis that the function of HgcA and HgcB may be linked to one carbon metabolism through the folate branch of the Wood-Ljungdahl pathway by providing methyl groups required for Hg methylation.

Anaerobic Mercury Methylation and Demethylation by *Geobacter bemidjiensis* Bem, and factors affecting methylmercury export and distribution

Baohua Gu, Xia Lu, Hui Lin, Alexander Johs, Aaron Jubb, Liyuan Liang, Eric Pierce
Oak Ridge National Laboratory, Oak Ridge, TN 37831

Subsurface Biogeochemical Research Program: ORNL Mercury SFA (PI: E.M. Pierce)

Contact: Baohua Gu (Gub1@ornl.gov)

Microbial methylation and demethylation are two competing processes controlling the net production and bioaccumulation of neurotoxic methylmercury (MeHg) in natural aquatic ecosystems. Although mercury (Hg) methylation by anaerobic microorganisms and demethylation by aerobic Hg-resistant bacteria have both been extensively studied, little attention has been given to MeHg degradation by anaerobic bacteria, particularly the iron-reducing bacterium *Geobacter bemidjiensis* Bem. We report, for the first time, that the strain *G. bemidjiensis* Bem can both methylate inorganic Hg and degrade MeHg concurrently under anoxic conditions. Results suggest that *G. bemidjiensis* cells utilize a reductive demethylation pathway to degrade MeHg, with elemental Hg(0) as the major reaction product, possibly due to the presence of homologs encoding both organo-mercurial lyase (MerB) and mercuric reductase (MerA) in this organism. Similarly as observed with the *G. sulfurreducens* PCA strain, *G. bemidjiensis* Bem cells can mediate multiple reactions including Hg/MeHg sorption, Hg reduction and oxidation, resulting in both time and concentration dependent Hg species transformations. Moderate concentrations (10–500 μM) of Hg-binding ligands such as cysteine enhance Hg(II) methylation but inhibit MeHg degradation. These findings indicate a cycle of methylation and demethylation among anaerobic bacteria and suggest that *mer*-mediated demethylation may play a role in the net balance of MeHg production in anoxic water and sediments.

Additionally, we studied the factors affecting MeHg export, sorption and distribution in cells, on cell surfaces, and in solution by known methylators including *G. bemidjiensis* Bem, *G. sulfurreducens* PCA, and *D. desulfuricans* ND132. We found that thiols, such as cysteine, can greatly facilitate desorption and export of MeHg, particularly by the PCA and Bem cells. In thiol-free assays, only a small percentage of the synthesized MeHg was found in solution, while most of the MeHg was associated with PCA or Bem cells, of which about 65-75% was sorbed on the cell surface and ~10-20% remained inside the cells. In comparison, ND132 cells were much more effective in excreting MeHg, with about 80% MeHg found in solution, leaving only a small percentage of the MeHg either sorbed on or remained inside the cells. These results indicate that MeHg export is bacteria-specific and is influenced by thiols, implicating important roles of complexing ligands, such as natural organic matter, in MeHg production and mobilization in the environment.

Insights into the Biochemistry of Microbial Mercury Methylation

A. Johs, R.C. Johnston, L. Liang, K. Neupane, J.M. Parks,
S.W. Ragsdale, K.W. Rush, S.J. Tomanicek, A.M. Whited, J. Zhou

Subsurface Biogeochemical Research Program: ORNL Mercury SFA (PI: E.M. Pierce)

Contact: Alex Johs (johsa@ornl.gov)

Microbial mercury methylation is an enzyme-catalyzed process carried out by certain anaerobic bacteria and archaea. The two-gene cluster *hgcAB* common is essential for mercury methylation. The genes encode a cobalamin-dependent protein, HgcA, and a ferredoxin, HgcB, which perform methyl transfer and cofactor reduction, respectively. Determining the interactions of HgcA and HgcB with other cellular components will provide greater understanding of methyl transfer mechanisms and the biochemical pathways involved in methylmercury production. The relationship between HgcA and HgcB and other metabolic pathways, such as one-carbon metabolism and electron transport, is of particular interest. These findings will provide essential data to inform metabolic and reactive transport models that can be used to predict mercury cycling from single organisms to ecosystems. Our studies will help understand the processes that control the fate and transformation of mercury in freshwater streams.

We have expressed HgcA and HgcB heterologously in *E. coli* and reconstituted both proteins with their respective cofactors. Changes in redox states of cobalamin and the 4Fe-4S clusters were characterized by UV-Vis spectroscopy. In collaboration with the Ragsdale lab at the University of Michigan, we are characterizing HgcA by EPR spectroscopy to investigate the coordination environment of the corrinoid cofactor in the Co(II) state. We are also investigating the transfer of electrons from pyruvate to HgcB facilitated by pyruvate ferredoxin oxidoreductase (PFOR). In an ongoing collaboration through a user proposal to EMSL (PNNL), we have collected two-dimensional NMR spectra to elucidate the structure of the cobalamin-binding domain of HgcA in solution. Insights obtained from these studies are complemented by structural bioinformatics to obtain a more complete picture at a systems level relevant to all Hg-methylating bacteria and archaea.

Exposure-time based approach for modeling mercury transport and transformation in low-order streams

Scott L. Painter, Scott Brooks, Guoping Tang

Environmental Sciences Division, Oak Ridge National Laboratory

The Mercury Science Focus Area at Oak Ridge National Laboratory recently initiated development of a new field-scale modeling framework for mercury transport and transformation in low-order streams. We describe an extensible framework that makes direct use of available field information and avoids the highly detailed site characterization that would be needed for detailed three-dimensional simulations. The approach is based on extending established travel-time based representations of watershed-scale transport to account for the time water is exposed to local biological “hot spots” for mercury methylation. In this framework, the three-dimensional concentration of mercury in various forms at any given location is controlled by the travel time of water parcels to that location from the mercury source and the exposure time, the time that water parcels are in contact with biologically active zones as they travel along their trajectories to the location of interest. In this conceptualization, computationally demanding three-dimensional reactive transport simulations are replaced with one-dimensional reactive transport simulations on an ensemble of trajectories through the stream channel, transient surface storage zones, and hyporheic zones, where each trajectory is characterized by travel time and exposure times. We are using the parallel, community code PFLOTRAN and are implementing a reactive transport system that includes mercury speciation in stream water, including complexation with natural organic material, sorption onto suspended solids, and diffusion-controlled exchanges between mobile water and periphyton biofilms where mercury methylation is assumed to occur (see companion Task 1 poster for details of those experiments). Potential strategies for informing the travel-time and exposure-time distributions based on field-scale tracer tests, parameter estimation, and eventually three-dimensional integrated surface-subsurface hydrology models will be summarized.

Probing Electrochemistry and Chemical Equilibria with Computational Chemistry: Corrinoids Related to Mercury Methylation

Jerry M. Parks,^{1,*} Ryne C. Johnston,¹ Alexander Johs,¹ Liyuan Liang,¹ Jeremy C. Smith,^{1,2} Stephen J. Tomanicek,² and Jing Zhou²

¹ Oak Ridge National Laboratory, ² University of Tennessee Knoxville

Subsurface Biogeochemical Research Program: ORNL Mercury SFA (PI: E.M. Pierce)

Contact: Jerry Parks (parksjm@ornl.gov)

Whether of anthropogenic or natural origin, mercury (Hg) is a highly mobile pollutant that can be transformed in the environment biotically by anaerobic bacteria and archaea and abiotically into the potent neurotoxin methylmercury (MeHg⁺), which, through bioaccumulation and environmental transport mechanisms, is a global concern. We previously identified the two-gene cluster solely responsible for biotic methylation and their gene products, HgcA, a transmembrane corrinoid (i.e., B12-binding) protein, and its corresponding ferredoxin, HgcB. HgcA was predicted to bind its corrinoid cofactor tail in a “Cys-on” configuration in which a strictly conserved Cys residue from HgcA is coordinated to Co. Our previous studies support our hypothesis that the electron-rich Co–S bond facilitates unprecedented methyl carbanion (H₃C:⁻) transfer to Hg^{II} rather than radical (H₃C[•]) or cation (H₃C⁺) transfer, both of which are ubiquitous across all life. We leverage our combined expertise in computational molecular modeling and experimental spectroscopic methods to provide atomistic insights into the corrinoid–protein interactions. Expanding upon our previously developed methods for computing accurate Hg–ligand binding free energies, here we report an accurate method for computing reduction potentials and related thermochemical properties for corrinoid cofactors using density functional theory (DFT). We additionally demonstrate the robustness of our approach to calculate UV-Vis and electron-paramagnetic resonance (EPR) spectra of model corrinoids in a range of coordination environments and oxidation states. Future studies will focus on transferring our improved method to model the speciation and fate of environmental Hg and relevant redox chemistry in natural aquatic systems. Central to this end of developing a more holistic model of mercury cycling *in silico*, we are also investigating passive transport across bacterial cell membrane models with molecular dynamics (MD) simulation approaches to understand cellular Hg loading and MeHg⁺ expulsion.

Biogeochemical Transformations at Critical Interfaces Science Focus Area: An Overview

Eric M. Pierce¹, Scott C. Brooks¹, Baohua Gu¹, Dwayne Elias¹, Jerry Parks¹, Alex Johs¹,
Cynthia Gilmour², and Judy Wall³

¹Oak Ridge National Laboratory, Oak Ridge, TN 37831

²Smithsonian Environmental Research Center, Edgewater, MD 21037-0028

³Biochemistry Division, University of Missouri

Subsurface Biogeochemical Research Program: ORNL Mercury SFA (PI: E.M. Pierce)

After making substantial progress over the past 6 years in understanding the processes that govern mercury transformation in contaminated systems, the ORNL SFA program is poised to make new transformational advances in mercury research and, more broadly, subsurface biogeochemistry in the program's subsequent phase. This next phase seeks to address the following science challenge and goal:

- **9-Year Science Challenge:** *Determine the coupled hydrobiogeochemical processes that control mercury fate and transformation in low-order freshwater stream systems and*
- **9-Year Science Goal:** *Process-rich predictive capability that integrates field, laboratory, and modeling studies of mercury fate and transformation dynamics across broad spatiotemporal scales in low-order streams.*

Low-order freshwater streams, such as EFPC (the project's representative use case), constitute nearly 90% of the total stream length in the United States and are the most frequently occurring stream type (>85%; Pierson et al. 2008). Furthermore, because of their low hydraulic radius (cross-sectional area and wetted perimeter) and low average water velocity, these stream systems have high water-sediment contact times, which promote in-stream biogeochemical cycling (Haggerty, Wondzell, and Johnson 2002). Numerous studies indicate that low-order streams play a dominant role in the flow, biogeochemistry, and water quality of downstream higher-order reaches (Alexander et al. 2007; Bernhardt et al. 2003; Waldron et al. 2009; Milliman and Syvitski 1992; Jeong et al. 2012). Additionally, these streams play a prominent role at the terrestrial-aquatic interface because they represent the first aquatic environment encountered by terrestrially derived materials (solutes and particles).

Developing a predictive understanding of mercury and trace metal transport and fate in environmental systems, such as terrestrial surface and subsurface ecosystems, is a formidable challenge that requires deciphering complex processes (i.e., physical, chemical, and biological), deconvoluting how these processes interact with one another, and understanding the factors that control system response over broad spatiotemporal scales.

Exchange and feedback processes at critical interfaces are central for determining fluxes, stocks, and transformation rates of key constituents that control mercury speciation, distribution, and bioavailability, such as oxygen, nutrients, and dissolved organic matter (DOM). Therefore, over the next 3 years, the ORNL SFA program will focus on: *Determining the fundamental mechanisms and environmental factors that control mercury biogeochemical transformations at key interfaces in terrestrial and aquatic ecosystems.* The research outlined in **Phase I** of the ORNL SFA plan comprises collaborative and complementary research activities that support four research thrusts: Ecosystem features influencing mercury transformation, Biogeochemical mechanisms controlling mercury uptake and methylation, Microbial community functions and geochemical influences on mercury transformations, and Molecular structure, dynamics, and mechanisms of mercury transport and transformations.

This presentation will summarize progress made to-date, which represents the initial 9-month period following the program's triennial peer review (April 2015) and acceptance of a renewal science plan, which occurred in August 2015 by the U.S. Department of Energy's (DOE) Office of Biological and Environmental Research.

PNNL ABSTRACTS

Field-scale Modeling of Hydrologic and Biogeochemical Dynamics in the Hyporheic Zone of the Columbia River along the Hanford Reach

PNNL SBR SFA (Laboratory Research Manager: Charlette Geffen)

Xingyuan Chen*¹ (Xingyuan.Chen@pnnl.gov), Xuehang Song¹, Glenn Hammond², James Stegen¹, and John Zachara¹ (PI)

¹*Pacific Northwest National Laboratory, Richland, WA*

²*Sandia National Laboratories, Albuquerque, NM*

Hydrologic and biogeochemical processes in the hyporheic zone of Columbia River along the Hanford reach are controlled by water level fluctuations in the river as a result of seasonal snowmelt and upstream dam operations, as well as local geologic structures and aquifer heterogeneity. Biogeochemical hot spots exist within a layer of alluvium (the hyporheic zone) that is situated between the riverbed and the adjacent unconfined aquifer. Monitoring of the microbial community within this zone along with water elevation, specific conductance, temperature and dissolved oxygen (DO) at different depths from the river bed (see poster by Stegen et al.) demonstrated a sharp gradient of dissolved oxygen within the first 40cm of alluvium. Laboratory experiments were conducted on fresh alluvial materials to identify key biogeochemical reaction networks within this carbon-containing layer (see poster by Liu et al.), including respiration, denitrification and nitrification. A field-scale hydro-biogeochemical model was formulated within PFLOTRAN based on a 2-D cross-section perpendicular to the river. The biogeochemical reaction network was adopted from laboratory experiments performed on sediments from the cross section. In-situ specific conductance observations from hyporheic zone piezometers were converted to groundwater fraction using a linear mixing model with river water and groundwater end-members. These were then assimilated within PFLOTRAN to estimate alluvium and aquifer permeabilities. DO profiles at 10cm and 40cm below the riverbed were used to estimate rate parameters for the reaction network. Effective model-data integration across scales allowed satisfactory simulation of this complex system. However, various challenges were revealed in attempting to model this complex and dynamic system. Additionally the need for more robust field monitoring of dissolved salts as tracers of water movement and source, and redox active solutes and dissolved gases as markers of biogeochemical reaction was affirmed as a priority for future field research.

Facies Delineation at Local and Reach Scales

PNNL SBR SFA (Laboratory Research Manager: Charlette Geffen)

Jason Hou* (Zhangshuan.hou@pnnl.gov), Chris Murray, Tim Scheibe, Evan Arntzen, Paul Thorne, Rob Mackley, Bill Nelson, James Stegen, Tim Johnson, Huiying Ren, Bill Perkins, Marshall Richmond, and John Zachara

Pacific Northwest National Laboratory, Richland, WA

Facies are elements of a sediment classification scheme that groups complex geologic materials into a manageable set of discrete classes. Facies classifications are arbitrary to a degree; their usefulness hinges on being able to distinctly relate facies type to quantitative properties needed for flow and reactive transport modeling (e.g., hydraulic properties, microbiologic characteristics). In the PNNL SFA, facies are being defined at multiple scales, providing a hierarchical structure for assigning multiscale model properties. At both reach and local scales, facies definitions are based on readily measured quantities that have adequate spatial coverage (e.g., stratigraphic units, grain size distribution, bathymetric and hydrodynamic attributes). Separate facies classifications have been defined in 1) the subsurface aquifer adjacent to and beneath the Columbia River (*subsurface facies*); and 2) the recent riverbed alluvial sediment (*riverine facies*).

Subsurface facies definitions and maps were based on pre-existing Hanford Site geologic maps. Hydraulic properties were related to facies type based on statistics of borehole measurements and pumping/slug test experiments. Subsurface facies and property maps are being used for local and reach scale modeling of hyporheic exchange, and are being refined as new data become available (e.g. hyporheic exchange observations from airborne electromagnetic and boat-based thermistor surveys). Riverine facies are less commonly studied than subsurface facies. Our riverine facies classification scheme is based on new measurements performed on freeze cores collected along the Columbia River shoreline. These were analyzed to quantify associations among microbial activity parameters (e.g., abundance of nitrite and carbon oxidizers), geochemical attributes (e.g., TOC, percentages of N/C/H), and physical properties. Multivariate data analyses indicated a strong relationship between physical and biogeochemical properties in the alluvial sediments. Mud and sand content, for example, were found to have strong associations with the abundance of nitrite and carbon oxidizing bacteria. Riverine facies are being refined and spatially mapped using river bathymetric attributes (e.g., slope, aspect, and local variability) and simulated hydrodynamic attributes (e.g., shear stress, flow velocity, river depth). Shear stress determines sediment transport and deposition and is associated with riverbed texture and sediment thickness. The spatial distribution of riverine facies will be further constrained using thermal imagery data and 3D time-lapse electrical resistivity tomography. The completed 3D distributions of riverine and subsurface facies and the corresponding flow, transport and biogeochemical properties will support parameterization of multiscale models of

hyporheic exchange between groundwater and river water and associated biogeochemical transformations.

Quantifying Reach-scale Dynamics of Groundwater-Surface Water Exchange and Land-Atmosphere Interactions along the Columbia River Shoreline through Model-Data Integration

PNNL SBR SFA (Laboratory Research Manager: Charlette Geffen)

Maoyi Huang^{1,*} (maoyi.huang@pnnl.gov), Tian Zhou¹, Jie Bao¹, Glenn Hammond², Xingyuan Chen¹, Gautam Bisht³, James Stegen¹, Evan Arntzen¹, Rob Mackley¹, Zhangshuan Hou¹, Heping Liu⁴, Justine Missik⁴, Zhongming Gao⁴, Eric Russell⁴, Christopher Strickland¹, William Perkins¹, Samuel Harding¹, Marshall Richmond¹, Scott Waichler¹, Scott Titzler¹, William Riley³, John Zachara¹

¹*Pacific Northwest National Laboratory, Richland, WA*

²*Sandia National Laboratories, Albuquerque, NM*

³*Lawrence Berkeley National Laboratory, Berkeley, CA*

⁴*Washington State University, Pullman, WA*

Lateral flow and transport between groundwater and river water through the subsurface interaction zone (SIZ) is a major pathway for energy, water, solute, and gas transfer between terrestrial and aquatic systems. Groundwater – surface water exchange is significant at multiple scales, but has been poorly quantified along large river reaches and has not been adequately resolved in Earth System Models (ESMs). Through an active collaboration among scientists at PNNL, SNL, LBNL, and WSU, the PNNL SBR-SFA has established a reach-scale research framework integrating high-fidelity computational tools with extensive surface and subsurface characterization and monitoring to assess the importance of SIZ at the reach scale. Specifically, the framework includes: (1) an integrated land surface and subsurface model enhanced with SIZ processes [i.e., CLM-PFLOTRAN] that is capable of quantifying water and solute exchanges in the SIZ and its impacts on land-atmosphere exchanges; (2) a computational fluid dynamics (CFD)-based approach for benchmarking hyporheic flow patterns under various flow conditions; (3) monitoring of land-atmosphere exchanges of water, energy, and CO₂ fluxes along the reach and across upland, riparian zone, and wetland locations; (4) characterization of surface/subsurface water conditions and groundwater-surface water exchange using in-situ boat-based observations.

A 7-km reach along the Columbia River shoreline has been selected to demonstrate the capability of this framework. Along the reach, subsurface and riverine facies are defined based on geo-stratigraphic and hydrodynamic attributes and their flow and transport properties are used for integrated simulations. A series of CFD simulations are first performed to understand hyporheic flow patterns and exchange rates under various flow conditions, which are validated by ground- and boat-based measurements. Idealized simulations are then conducted to isolate the roles of geomorphological features such as river bathymetry, islands and bars in modulating hyporheic flow patterns and exchanges. Lastly, CLM-PFLOTRAN simulations, benchmarked by the CFD simulations, are being performed for a period of five years (2010-2015) spanning high and low flow conditions to quantify the inter-annual variability of hyporheic exchange and its role in modulating land-atmosphere interactions. The research framework, capable of quantifying hyporheic and land-atmosphere exchanges through model-data integration, establishes a solid foundation for better understanding the spatial and temporal dynamics of biogeochemical cycling and biogenic gas generation in the SIZ, and their impacts on and regulation by the changing water cycle and climate. Subsequent research will integrate a multi-scale facies definition (e.g., Hou et al) to extend the integrated modeling approach to the 75 km Hanford Reach, a typical scale relevant to ESM development in DOE projects.

Model-driven hydro-geophysical characterization of the groundwater-surface water interaction zone

Tim Johnson¹ (tj@pnnl.gov), Xingyuan Chen¹, Xuehang Song¹, Glenn Hammond²,
and James Stegen¹

¹*Pacific Northwest National Laboratory, Richland, WA*

²*Sandia National Laboratories, Albuquerque, NM*

Biogeochemical activity in the 300 Area groundwater surface water interaction zone (SIZ) is highly influenced by stage-driven river water intrusion. Columbia River water supplies oxygen and select nutrients whereas groundwater supplies nitrogen that collectively regulate the biogeochemical function of microbial communities within the SIZ (see posters by Stegen et al., and Roden et al.). Because of this, the capability to predict biogeochemical activity in terms of contaminant behavior and carbon cycling within the SIZ depends critically on the capability to predict groundwater-surface water mixing dynamics (see poster by Chen et al.). To do so, the hydrogeologic structure that governs flow and transport within the SIZ must be adequately constrained.

We are using flow and transport calculations, coupled with geophysical simulations, to guide geophysical experiments aimed at constraining the hydrogeologic structure of the SIZ. In the first step, a conceptual flow and transport model of the SIZ is used to identify critical features that must be constrained in order to accurately predict biogeochemical processes. In the second step, coupled hydro-geophysical simulations are used to design and assess the feasibility of using geophysical data to inform the flow model concerning the critical features identified in the first step. In the third step, field geophysical data are collected, using optimized data collection strategies identified in the second step. In the fourth step, the geophysical data are used to constrain the critical features identified in step 1. Step four is accomplished by 1) incorporating geologic contact information identified by geophysical images into the flow model discretization, or 2) using time-lapse geophysical measurements directly in a coupled hydrogeophysical inversion. In this poster, we demonstrate the approach using high resolution underwater spectral induced polarization imaging to constrain riverbed structure, which has been shown to significantly impact groundwater-river water interaction (Hammond et al., 2010). We also demonstrate the approach using underwater, high resolution, time-lapse electrical resistivity data to inform the flow model of groundwater surface-water interaction near the riverbed, to approximately 5m depth.

Functional Enzyme-based Metabolic Models for Simulating Biogeochemical Processes

PNNL SBR SFA (Laboratory Research Manager: Charlette Geffen)

Chongxuan Liu* (Chongxuan.liu@pnnl.gov), Hyun-Seob Song, Jeremy Zucker, Minjing Li, Yuqian Gao, Weijun Qian, Liang Shi, Yuanyuan Liu, William Nelson, Jim Fredrickson, and John Zachara

Pacific Northwest National Laboratory, Richland, WA

Microbially-mediated biogeochemical processes are regulated by enzymatic activities that control the biogeochemical transformation of carbon, nitrogen, and other elements in natural environments. However, enzymes are often replaced using biomass or functional genes as surrogates in biogeochemical models because the quantification of specific enzyme concentrations in environmental samples is difficult. In this research, we developed a signature peptide-based technique that can efficiently and directly quantify multiple functional enzymes and their dynamics in sediments. This new technique was then used to investigate the correlations between functional enzyme concentrations and biogeochemical species concentrations during nitrate bioreduction in Columbia River hyporheic zone sediments from the Hanford site. A functional enzyme-based metabolic model was developed to describe multi-component biogeochemical processes based on the correlation results, measurements of the corresponding functional genes, and a theoretical analysis of metabolic energetics. The model divides the microbial community into multiple functional entities, each characterized by a specific functional enzyme informed by environmental genomics. The functional enzymes explicitly link microbial metabolism with the biogeochemical reaction network. The resulting metabolic model was implemented using three alternative system-scale modeling approaches that differ in their conceptualization of functional enzyme production and reactivity in natural systems. The first approach uses the inhibition concept derived from experimental observations that some enzyme activities will be inhibited in the presence of certain types of biogeochemical species (e.g., O_2). The second approach uses the cybernetic concept that provides a rational description of the dynamic regulation of enzyme syntheses and activities based on control theory. The third approach uses the maximum entropy production principle derived from nonequilibrium statistical mechanics fluctuation theorem to regulate the evolution of microbial community functions and biogeochemical reactions. These approaches are currently being tested using the experimental data to evaluate their effectiveness and predictability. The metabolic model and system-scale modeling approaches provide a framework for describing the coupled evolution of microbial community functions and the biogeochemical transformations of organic carbon, nitrate, and contaminants in hyporheic zone sediments at both laboratory and field scales.

Fine Scale Biogeochemical Processes in Hyporheic Zone Sediments

PNNL SBR SFA (Laboratory Research Manager: Charlette Geffen)

Yuanyuan Liu, Chongxuan Liu* (Chongxuan.liu@pnnl.gov), Fen Xu, Yunde Liu, Liang Shi, William Nelson, Jim Fredrickson, John Zachara, Weijun Qian, Minjing Li, Ailan Yan

Pacific Northwest National Laboratory, Richland, WA

A series of experiments and model simulations were performed to derive kinetic models and parameters for describing the biogeochemical transformations of organic carbon, nitrate, and contaminant (Cr) in Columbia River hyporheic zone sediments. Denitrification of nitrate to nitrite and gaseous N_2O and N_2 ; direct nitrate reduction to ammonium (DNRA); nitrification from ammonium to nitrate; and anaerobic ammonium oxidation (Anammox) were all observed in the hyporheic zone sediments. The relative importance of these multiple processes to nitrate transformation was influenced by contact water chemical composition, fluid residence time, and ion exchange reactions. Dissolved and sediment-associated organic carbon (OC) chemical properties including speciation, nominal oxidation state, and double bond counts changed significantly during nitrate transformation in response to the changes in contact water chemical composition. A reaction network has been established based on these findings to describe nitrate- and, more generally, N-transformation in the sediments. These results, combined with functional gene, enzymes measurements, and microbial community analysis, will be used to evaluate enzyme-based biogeochemical models to describe the evolution of microbial community functions and biogeochemical process kinetics.

Experiments and modeling simulations were also performed using the Cr redox reaction as a probe to investigate the redox properties of the hyporheic zone sediments. Kinetic studies indicated that Cr(VI) can be reduced to poorly soluble Cr(III) with a reduction rate that correlated with the sediment Fe(II) concentration. The reduced Cr was stable in presence of O_2 and Mn oxides under circumneutral pH conditions. Microbial reduction of the sediments promoted by native OC can further enhance the redox capacity and the rate of Cr reduction. A reaction network linking Cr(VI) reduction with Fe(II) oxidation, the production of biogenic Fe(II) coupled with OC oxidation, and abiotic oxidation of Fe(II) by river water oxygen was developed and applied to simulate coupled biotic and abiotic reactions in the hyporheic zone under dynamic hydrological conditions. The results provide important insights to the functioning of the hyporheic zone as a redox barrier for Cr sequestration. The reaction network and associated kinetic parameters for N, Fe, and Cr redox transformations coupled with OC speciation forms the basis for an integrated multi-component, biogeochemical kinetic model applicable to the Columbia River hyporheic zone and up-scaled domains of the Hanford Reach.

Composition and Metabolic Activity of Columbia River SIZ Microbial Communities in Relation to Habitat and DOC Source

PNNL SBR SFA (Laboratory Research Manager: Charlette Geffen)

Eric Roden^{*1} (eroden@geology.wisc.edu), Noah Stern¹, James Stegen², Evan Arntzen² and David Kennedy²

¹*University of Wisconsin, Madison, WI*

²*Pacific Northwest National Laboratory, Richland, WA*

Hyporheic zone exchange of dissolved organic carbon (DOC) and nutrients between groundwater and river water plays a critical role in biogeochemical cycling within the Columbia River (CR) subsurface interaction zone (SIZ). Fluid exchanges may set limits on absolute rates of bulk carbon and nutrient processing, and impose deterministic selection on attached microbial communities that are adapted to utilize dynamically changing DOC sources. This study examined the response of attached microbial communities that developed in situ in three different zones (groundwater, hyporheic, and river water) within the SIZ to “cross-feeding” with DOC and other nutrients in either groundwater (GW) or river water (RW). Our working hypothesis was that in situ exposure history would dictate attached microbial community composition and physiological potential, thereby influencing rates of microbial metabolism. Sterile, organic-free Hanford sand was incubated in situ in 300 Area Hanford Formation groundwater, in piezometers embedded a few meters into the riverbed, or on the surface of the armored (pebble) layer of the riverbed itself (covered by dark screening to prevent illumination). Following a six-week period of in situ incubation and microbial colonization, the sands were retrieved and suspended in RW, GW, or artificial (organic-free) versions of these two fluid sources. Measurements of microbial biomass (ATP content), community structure (16S rRNA gene sequencing), and respiratory activity (aerobic microbial reduction of resazurin to resorufin), were made over a period of six weeks, with weekly exposure of the sands to fresh, sterile-filtered feed solutions. In contrast to expectations, the major observation was that the riverbed incubated sand had much higher biomass and respiratory activity, as well as a very different community structure, compared to the groundwater and piezometer incubated sand. Specifically, 16S rRNA gene analysis of community composition revealed that the most abundant taxa in the riverbed incubated sand were not prokaryotic organisms but rather the chloroplasts of diatoms. These results provide evidence for transport of diatom biomass into the riverbed. Analogous results were obtained in a repeat of the cross-feeding experiment, and in experiments designed to test whether DOC released from riverbed sediments could stimulate metabolism of colonized sand materials. A key implication of these results is that deposition of fresh, labile particulate organic carbon to the river bed leads to relatively high microbial biomass and metabolism by attached microbial communities. It also likely leads to release of DOC which may enter the SIZ via hyporheic zone exchange to stimulate microbial activity therein.

Hybrid Multiscale Simulation of Hydro-Biogeochemical Processes in the Groundwater-Surface Water Interaction Zone

PNNL SBR SFA (Laboratory Research Manager: Charlette Geffen)

Tim Scheibe*¹ (Co-PI; tim.scheibe@pnnl.gov), Xiaofan Yang¹, Xuehang Song¹, Glenn Hammond², Xingyuan Chen¹, Ilenia Battiato³, Svyatoslav Korneev³, and John Zachara¹ (PI)

¹*Pacific Northwest National Laboratory, Richland, WA*

²*Sandia National Laboratories, Albuquerque, NM*

³*San Diego State University, San Diego, CA*

The PNNL SFA is developing a predictive understanding of the groundwater-surface water interaction zone (termed the subsurface interaction zone, SIZ). A key element of this research is a multiscale modeling framework that facilitates the integration of new mechanistic understanding from fine-scale controlled laboratory studies (bottom-up) with diverse field-scale observations (top-down). Our hybrid multiscale modeling approach couples models of fluid flow and biogeochemical transport formulated at various scales (e.g., pore, darcy, and field scales) to provide increased process fidelity when and where needed (according to well-defined model error criteria) while maintaining computational feasibility over a large domain. The SIZ plays an important role in natural ecosystems as it functions as an interface between terrestrial, subsurface and aquatic systems. Locally it regulates the mixing of nutrients that control biogeochemical transformations of solutes of both groundwater and riverine origin. Subsurface heterogeneity can give rise to local hotspots of microbial activity that are important to system function yet difficult to resolve computationally. To address this challenge, we are testing our hybrid multiscale approach using the same field-scale model domain utilized in SFA Task 2 field and modeling studies (Stegen et al. poster; Chen et al poster). The region of interest intersects the aquifer and the river and contains a contaminant plume. However, biogeochemical activity appears to be highest in a thin zone (river alluvium layer, <1 m thick) immediately underlying the river where organic matter accumulates. It is not computationally feasible to resolve the full macroscale domain at the fine resolution potentially needed in the alluvium layer, and the multi-component reaction network applicable in the alluvium layer is more complex than is needed in the rest of the macroscale domain. Hence, the hybrid multiscale approach is used to couple high-fidelity simulations of alluvium layer processes with coarsely-resolved simulations of the larger domain. Models at both scales are simulated using the PFLOTRAN code in a series of increasingly complex system conceptualizations: 1) Homogeneous alluvium and uniform biogeochemical reaction network (comparable to the Task 2 single-scale model); 2) Heterogeneous alluvium and uniform biogeochemical reaction network; and 3) Heterogeneous alluvium and more complex biogeochemical reaction network in alluvium layer. Through this series of numerical experiments, we are able to quantify the computational costs and differences in model

predictions associated with the multiscale hybrid method, and to quantify the potential impacts of biogeochemical hotspots in the alluvium layer on system behavior.

Linkages among Geophysical Facies, Microbial Composition, Biogeochemical Rates, and Seasonal Hydrology in the Hyporheic Zone

PNNL SFA (Laboratory Research Manager: Charlette Geffen)

James Stegen* (James.Stegen@pnnl.gov), Evan Arntzen, Alex Crump, Sarah Fansler, Jim Fredrickson (Co-PI), Emily Graham, Jason Hou, Dave Kennedy, Bill Nelson, Tom Resch, and John Zachara (PI)

Pacific Northwest National Laboratory, Richland, WA

The hyporheic zone is a critical ecosystem transition that links terrestrial, aquatic, and subsurface domains. To understand connections among physical, microbial, and biogeochemical components of the hyporheic zone, we obtained approximate 0.5 m freeze-cores along the Columbia River in the Hanford 300 Area and performed geologic, molecular, and microbial assays. Relationships among these data types were assessed using multivariate statistics; mud and sand content were found to be the primary drivers of microbial community attributes (in particular, of nitrite and carbon oxidizers). Microbial community analysis revealed an abundance of nitrifying Archaea (*Thaumarchaea*) and an absence of nitrifying Bacteria. Network analysis revealed significant negative correlations between sand content and some statistical modules of microbial taxa, perhaps indicating the importance of pore water residence time on community composition. A similar set of microbial modules was positively correlated with total organic carbon. One such module that also positively correlated with aerobic metabolic rates was dominated by *Thaumarchaea* and *Nitrospira*, suggesting that ammonia oxidation--instead of respiration--was the dominant aerobic process at the time of sample collection. We further examined temporal changes in hyporheic microbial community structure and activity through repeated sampling of attached and pore water microbial communities across a spatial gradient. We found that microbial communities remained distinct in river, hyporheic, and inland zones across seasonal variation in hydrologic mixing conditions. One factor that resulted in distinct communities across the three zones was temperature-driven increases in microbial species richness in the hyporheic zone. We employed a combination of null modeling and multivariate statistics to show that the relative importance of ecological selection and dispersal varied across environments (e.g., pore water vs. attached) and across geographic zones. Our results also indicated that while selection imposed short-term constraints on microbial community structure, hyporheic sediment communities did not respond to short-term hydrologic variation. Importantly, we demonstrated that the influence of selective pressures varied with phylogenetic affiliation, which may have been responsible for seasonal increases in *Thaumarchaea* and aerobic activity. Taken together, our results elucidate spatiotemporal shifts in the composition and activity of hyporheic microbial communities across sedimentary geochemical gradients as well seasonal gradients in pore water environments that correlate with the contribution of *Thaumarchaea* to aerobic processes.

Pacific Northwest National Laboratory SFA: Hydro-Biogeochemical Process Dynamics in the Groundwater-Surface Water Interaction Zone

PNNL SBR SFA (Laboratory Research Manager: Charlette Geffen)

John Zachara*¹ (PI; john.zachara@pnnl.gov), Jim Fredrickson¹ (Co-PI), Tim Scheibe¹ (Co-PI), Xingyuan Chen¹, Glenn Hammond², Maoyi Huang¹, Jason Hou¹, Chongxuan Liu¹, Chris Murray¹, Hyun-Seob Song¹, and James Stegen¹

¹*Pacific Northwest National Laboratory, Richland, WA*

²*Sandia National Laboratories, Albuquerque, NM*

The PNNL SFA is developing a predictive understanding of the groundwater-surface water interaction zone (termed the subsurface interaction zone, SIZ). The SIZ is a ubiquitous and biogeochemically active domain within river corridor systems that controls contaminant, nutrient, and biogenic gas releases to surface waters. It is hydrologically dynamic, vulnerable to the effects of climate change, and includes but is not limited to the hyporheic zone where gradients in water composition and dissolved oxygen drive complex biogeochemical processes. Active carbon and nitrogen cycling occurs within the SIZ that are key to surface water quality and gas exchanges with the atmosphere. Using the 75 km Hanford Reach of the Columbia River as our research domain, overarching science questions on the function and impact of subsurface interaction zone are driven down from the reach scale to focus lower-scale scientific hypotheses and comprehensive field studies at the kilometer scale and below on essential system attributes, behaviors, and mechanisms for robust process model development. These questions relate to: i) hyporheic exchange flows and groundwater-surface water mixing, ii) residence times and pathways of different water sources, and biogeochemical processes and fluxes, iii) the composition and biogeochemical function of microbial communities across geochemical and temperature gradients, and iv) the nature, speciation, and energetics of organic carbon driving biogeochemical processes. A facies-based, multiscale simulation framework is being established to connect biogeochemical transport models across scales while preserving robust process descriptions derived at local field sites along the Hanford Reach and with field derived sediments in the laboratory. New microbial ecological models are being formulated and tested to translate microbial community composition and function into biogeochemical process rates controlled by environmental conditions. Our research on the subsurface interaction zone will provide essential knowledge and relevant models for rivers worldwide that flow through glacio-fluvial aquifers and for catchments with coarse-grained sediments that are vulnerable to climate change.

SLAC ABSTRACTS

SLAC SFA: Mechanistic linkages between floodplain critical element and contaminant redox cycles

Program Affiliation: Subsurface Biogeochemical Research

Lead PI: John R. Bargar¹

Authors: Vincent Noël¹, Kristin Boye², Albert Müller², Sharon E. Bone¹, Emily Cardarelli², Juan S. Lezama-Pacheco², Pierre Lefebvre³, Kenneth H. Williams⁴, William L. Dam⁵, Ray Johnson⁵, Ravi Kukkadapu⁶, Malak Tfaily⁶, Rosalie K. Chu⁶, Ljiljana Pasa-Tolic⁶, Alfred M. Spormann², Scott Fendorf², and John R. Bargar¹

Affiliations: ¹SLAC National Accelerator Laboratory, ²Stanford University, ³Ecole Normal Supérieure de Paris, ⁴Lawrence Berkeley National Laboratory, ⁵DOE Office of Legacy Management, ⁶Environmental Molecular Sciences Laboratory

Organic-rich sulfidic sediments in the uranium-contaminated floodplain at the DOE site in Rifle, Colorado, exhibit U(IV) concentrations 100-fold higher than the local background. Our prior studies led to the hypotheses that: 1) these naturally reduced zone (NRZ) sediment bodies are general features of floodplains and *regionally* accumulate uranium in the upper Colorado River Basin (CRB); 2) NRZs are regionally important regulators of biogeochemical critical element (BCE, e.g. C, N, S, Fe) cycling, and 3) Uranium fate is tightly linked to BCE redox cycling in NRZs. The SLAC-SFA is investigating the validity of these hypotheses through in-depth molecular analyses of BCE and contaminant chemistry in sediment cores at fine spatial resolution.

In the past year, we have completed new NRZ sediment and pore water sampling activities at Rifle, Naturita, and Grand Junction CO; Shiprock, NM; and Riverton, WY. This work has confirmed that NRZs are common features of these floodplains and that they harbor large U and organic C inventories. Using spectroscopic methods (including X-ray absorption spectroscopy, Mössbauer spectroscopy, X-ray diffraction, and Fourier transform ion cyclotron resonance mass spectrometry) combined with chemical extraction and U isotopic signatures, we have established and compared depth profiles of detailed speciation information for U, Fe, S and C from all five floodplains. This work shows that there is an overall regional inverse correlation between the nominal oxidation state of carbon (NOSC) and increasing sulfide and U content, providing a mechanistic molecular explanation for the tight coupling between U, S and C cycling within NRZ sediments. The NOSC of soluble organic compounds in U-enriched NRZs is close to or below the thermodynamic limit for microbial respiration with sulfate as the terminal electron acceptor, indicating that U is retained here because of its higher thermodynamic favorability in supporting microbial respiratory growth. Combined with sediment pore water and microbial respiration data, this information is allowing us to construct a regional conceptual model of the ecosystem biogeochemical functions of NRZs in upper CRB floodplains.

To develop a more detailed mechanistic understanding of the links between organic matter decomposition and different element cycles, we are further examining the syntrophic coupling of fermentation to anaerobic respiration on solid phase substrates. This work is providing essential knowledge about the relevance of carbon substrate chemistry, spatial separation and electron acceptor availability for the rate and mode of coupled, microbially mediated redox transformations.

SLAC SFA: Coupled cycling of organic matter, uranium, and biogeochemical critical elements in subsurface systems

Program Affiliation: Subsurface Biogeochemical Research

Lead PI: John R. Bargar¹

Authors: John R. Bargar¹, Scott Fendorf², Chris A. Francis², Kate Maher², and Alfred Spormann²

Affiliations: ¹SLAC National Accelerator Laboratory, ²Stanford University

Organic-rich sulfidic sediment lenses hosting relatively high uranium concentrations have been observed at DOE's Rifle, CO site. Subsequently we have observed similar bodies at other uranium-contaminated DOE sites in the upper Colorado River Basin (CRB), including Grand Junction and Naturita, CO; Shiprock, NM; and Riverton, WY. These naturally reduced zones (NRZs) also store large inventories of nutrients and biogeochemical critical elements (BCEs, including C, N, S, and Fe) and they lie within or below the zone of annual groundwater table fluctuations where they are subject to radical hydrologic changes from saturation to highly unsaturated. Thus, NRZs constitute a class of regionally-important biogeochemical hotspots that have the potential to modify the mobility of nutrients, BCEs, uranium, and other contaminants within otherwise oxic nutrient-poor floodplain systems. Large-scale ecosystem perturbations such as extended drought and flooding have the potential to alter NRZ biogeochemistry and to discharge contaminant and nutrient loads to connected ground and surface water systems. There is concern that NRZs are contributing to uranium plume persistence regionally or could do so in the future.

We are investigating the fundamental hydro-biogeochemical mechanisms by which organic matter in NRZs mediates the speciation, behavior, and fluxes of BCEs and uranium across a range of scales, from molecular to regional. Our goal is to identify, interrogate, and model critical processes in these subsurface ecosystems to improve BER's computational subsurface research capabilities and to anticipate impacts to floodplain systems and society under changing climate conditions. Questions being investigated include: (i) What are the physical and hydro-biogeochemical characteristics of NRZs? (ii) What biological, kinetic, and thermodynamic factors control the speciation and behavior of uranium and BCEs? (iii) How do NRZs interact with surrounding floodplain aquifers? (iv) How does microbial N cycling mediate redox conditions? and (v) What are the mechanisms and rates of uranium release to surrounding aquifers?

We are using an integrated suite of approaches to address these questions, including field-scale investigations at sites across the upper CRB coupled to laboratory-based molecular scale investigations using x-ray absorption spectroscopy, x-ray, electron, and isotope imaging, molecular microbial ecology, electrochemistry, and stable isotope techniques. Over the past year, these investigations have advanced our knowledge of NRZ biogeochemistry and are leading to new process-level models to understand their function at floodplain to regional scales.

Program Affiliation: Subsurface Biogeochemical Research

Lead PI: J. R. Bargar¹

Co-authors: S.E. Bone¹, M. E. Jones², K. Boye², V. Noel², E. Cardarelli², W.L. Dam³, R.H. Johnson⁴, J. Dynes⁵, J. Cliff⁶, S. Fendorf²

Affiliations: ¹SLAC National Accelerator Laboratory, ²Stanford University, ³U.S. DOE Office of Legacy Management, ⁴Navarro Research and Engineering, Contractor to the U.S. DOE Office of Legacy Management, ⁵Canadian Light Source, ⁶Environmental Molecular Sciences Laboratory

The fate and transport of uranium is largely dictated by oxidation state. Within floodplains, physical heterogeneity produces organic-rich, sulfidic, fine-grained zones within otherwise organic-poor siliciclastic aquifers. Reduction of U(VI) in these naturally reduced zone (NRZ) sediments leads to the accumulation of non-crystalline U(IV), which can subsequently resupply U to contaminated floodplain aquifers. Numerous questions remain unaddressed regarding U reduction under these dilute, organic-rich natural conditions. The relative importance of bacterial versus abiotic reduction is unresolved. So-called “non-crystalline” U(IV) species are poorly characterized, and the mechanistic “switch” leading to crystalline and non-crystalline products is unknown. We examined U(VI) reduction pathways and products in a model system designed to emulate key NRZ conditions (nutrient limitation, natural consortia, organic sorbents, and dilute U(VI)). Uranium(VI) was reduced by dissimilatory microbial communities, whereas reduction of U(VI) by aqueous S(-II) was not appreciable. Uranium(IV) adsorption complexes were the dominant products at U(VI) concentrations $\leq 10 \mu\text{M}$, indicating that U(IV) complexes likely prevail at many contaminated sites that exhibit similar or lower U concentrations. Precipitation of uraninite at higher U(VI) concentrations is consistent with thermodynamics.

We used cyclic voltammetry to examine the effects of pH, and concentrations of uranium, carbonate, and calcium on the redox transitions of the uranyl ion. Redox potentials of U(VI) to U(V), U(V) to U(IV), and U(IV) to U(III) transitions between pH 3-8 were determined. Similar to bacterial and Fe(II) reduction, Ca within the dicalcium complex blocks the electron transfer pathway, illustrating the utility of electrochemistry for resolving redox reaction mechanisms.

Oxidant incursions driven by seasonal water table fluctuations drive uranium transformation and release from NRZs. We posit that nitrate, as well as oxygen, are important oxidants. To test this hypothesis, we examined how diffusion-limited mass exchange between NRZ sediments (Riverton, WY site) and groundwater impacted the magnitude and rate of U(VI) release. We employed diffusion-limited flow reactors under anoxic (control), oxygenated (250 μM O₂) and elevated nitrate (1 mM) conditions. Although DO led to sustained U release from the sediments, nitrate-induced oxidative release was suppressed by sulfate reduction. Sedimentary organic matter in the NRZ sediments supports microbial respiration with SO₄²⁻ at attenuated U(VI) oxidation, although denitrification co-occurred. Our work demonstrates that the magnitude and duration of oxidative U release from NRZ sediments depends on the interplay between terminal electron acceptor (TEA) supply (O₂, NO₃⁻, or SO₄²⁻) and the availability of organic matter for microbial respiration with different TEAs.

SLAC SFA: Diversity and biogeography of subsurface nitrogen-cycling communities at uranium-contaminated DOE legacy sites in the upper Colorado River Basin

Program Affiliation: Subsurface Biogeochemical Research

Lead PI: John R. Bargar¹ (bargar@slac.stanford.edu)

Co-authors: Emily Cardarelli² (ecardare@stanford.edu), Kristin Boye² (kboye@stanford.edu), William L. Dam³ (william.dam@lm.doe.gov), Ray H. Johnson⁴ (ray.johnson@lm.doe.gov), Kenneth H. Williams⁵ (khwilliams@lbl.gov), Christopher A. Francis² (caf@stanford.edu)

Affiliations: ¹SLAC National Accelerator Laboratory, ²Stanford University, ³U.S. DOE Office of Legacy Management, ⁴Navarro Research and Engineering, Contractor to the U.S. DOE Office of Legacy Management, ⁵Lawrence Berkeley National Laboratory

The products of nitrification (NO_2^- , NO_3^-) and denitrification (NO_2^- , NO , N_2O) have been shown to impact the fate and mobility of uranium (U) at contaminated DOE legacy sites. By converting ammonia released by the decomposition of organic matter to nitrite and nitrate, nitrification effectively links the most reduced and oxidized pools of nitrogen in the environment. Under anoxic conditions, denitrification converts these nitrogen oxides to gaseous forms, which are lost from the system. Furthermore, the cycling and bioavailability of N in subsurface ecosystems is frequently coupled to redox cycles of other biogeochemical critical elements (e.g. C, S, Fe). Despite its importance, little is known regarding the diversity, abundance, and activity of N-cycling communities in such ecosystems.

We have examined ammonia-oxidizing and denitrifying microbial communities at multiple U-contaminated legacy sites in the Upper Colorado River Basin (CRB). Cores (~5-10 m deep) were collected from the alluvial floodplain at Naturita, CO, and Grand Junction, CO, by Geoprobe coring, and from Rifle, CO, Shiprock, NM, and Riverton, WY, by sonic rotary drilling. To examine the diversity and structure of the ammonia-oxidizing communities within and across these sites, a combination of sequencing and quantitative PCR of the *amoA* gene (encoding the α -subunit of ammonia monooxygenase) was applied to more than 300 sediment samples. This resulted in an extensive database of >1500 *amoA* sequences from both ammonia-oxidizing archaea (AOA) and bacteria (AOB). Interestingly, AOA *amoA* abundances ($8 \times 10^2 - 5 \times 10^8$ copies per g sediment) are consistently higher than those of AOB ($1 \times 10^2 - 5 \times 10^6$ copies per g sediment), suggesting that AOA play a prominent biogeochemical role in these sediments. Denitrifying communities are also being examined within naturally-reduced zone sediments using the functional genes *nirK* and *nirS* (encoding dissimilatory nitrite reductase) as molecular markers.

To better understand N-cycling microbial community dynamics in U-contaminated field sediments, flow-through columns were used to provide time-resolved DNA/RNA samples coupled to detailed geochemical analyses. Nitrate, nitrite, and oxygen were added to influents to study their impact on uranium oxidation. N-cycling microbial communities were characterized as a function of depth, distance from the sediment-water interface, and through time, to determine where and to what extent uranium oxidation by these oxidants occurs. Ultimately, this combination of field- and laboratory-scale approaches will provide critical insights into the interplay between microbial N-cycling and U mobility in the subsurface.

SFA - TES ABSTRACTS

Minerals control soil decomposition and organic carbon accumulation over decadal timescales: A modeling analysis

Authors: RZ Abramoff, J Tang, K Georgiou, MS Torn, WJ Riley

Soil carbon (C) is the largest actively cycling terrestrial pool of C with a mean residence time that can exceed 10,000 years. The formation and release of soil C is controlled by biogenic processes (e.g., plant allocation to litter and root exudates, microbial growth and metabolism) and chemical processes (e.g., sorption to minerals, temperature, water availability), and thus the rate of decomposition can change non-linearly over time as a result of multiple constraints. Heterotrophic decomposition releases organic C back into the atmosphere as carbon dioxide and is therefore an important feedback to global change. Terrestrial biosphere models of soil decomposition generally use a linear turnover rate for 1–9 soil C pools that vary in lability, assuming that the persistence of soil organic carbon (SOC) is due to intrinsic chemical recalcitrance. However, recent work has suggested sorption to minerals as an alternative mechanism for SOC protection. This paradigm is supported by experiments that show that old SOC can have low thermodynamic stability and turn over quickly with warming or other disturbance.

We performed a modeling experiment using a model that explicitly represents microbial activity, mineral sorption, nutrient availability, and water stress as potential constraints on the rate of decomposition and the long-term SOC stock. We spun-up eight model runs for 1000 years using a range of mineral surface area derived from literature. We then ran each model for 1–50 years over a range of plant inputs and climatic conditions to test for the relative effect of mineral, plant, and climate drivers on seasonal- and decadal-scale SOC storage. We found that sorption to mineral surfaces was an important control over decadal SOC stock dynamics while changes in temperature and water content had a smaller relative effect. The magnitude and stoichiometry of plant inputs affected decomposition rates and SOC stocks on seasonal and decadal scales. On seasonal timescales, decomposition rate was sensitive to microbial physiology parameters such as maximum growth rate, but on decadal timescales microbial growth was limited more by substrate supply than intrinsic rate. The model output coincided with published observed relationships between SOC stocks, geochemical variables, and climate from multiple ecosystems, suggesting that mineral sorption is an important long-term control on soil C stock.

Toward a More Nuanced Understanding of Carbon Dioxide Emissions from Fossil Fuel Combustion: Highlights of the Last Year of TES Funding

R. J. Andres¹, A.W. King²

¹Carbon Dioxide Information Analysis Center, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6290 [USA](#)

²Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6301 [USA](#)

e-mail: andresrj@ornl.gov

Creating gridded uncertainty maps of carbon dioxide emissions from fossil fuel combustion was the focus of much of the last year. Since physical measurements at the appropriate spatial and temporal scales do not exist, all current global maps of fossil fuel carbon dioxide emissions use one or more proxies to distribute emissions. These proxies introduce additional uncertainty into these maps, beyond the uncertainty associated with the undistributed emissions magnitude. This uncertainty, gridded at the same spatial and temporal scales as the emission magnitude maps, includes contributions from the spatial, temporal, proxy, and magnitude components used to create the magnitude map of FFCO₂ emissions. This work follows on from the global uncertainty analysis published in 2014 (Andres et al., 2014, *Tellus B*, 66, 23616. doi:10.3402/tellusb.v66.23616). The gridded uncertainty manuscript will be submitted for publication soon.

In addition to the uncertainty focus, TES funding contributed to revisions and the addition of another year to the CDIAC fossil fuel carbon dioxide time series. The current time series now ends in 2011 and emission year 2012 is now being investigated. These data are available annually and monthly, in tabular form and gridded at one degree scale.

TES funding is also contributing to a better understanding of the influence of changing fossil-fuel ¹³C emissions on ¹³C tracer experiments at the SPRUCE site. This requires a highly precise and accurate model of ¹³C photosynthetic fractionation and fixation. Using the TES-SFA's functional unit testing framework, ecosystem-wide process representations of ¹³C fractionation and fixation for incorporation into CLM-SPRUCE and other models are being examined, beginning with the Sun and Gu photosynthesis model that incorporates mesophyll conductance in isotopic discrimination. Uncertainty in the parameters of this sophisticated model will propagate into uncertainty in simulated biomass ¹³C. The functional unit testing allows exploration of this uncertainty and the consideration of alternative formulations which may be less precise in principle but have smaller associated parametric uncertainty.

Peer-reviewed publication of this work continues. Since the last TES presentation one year ago, TES funding has contributed to four major publications (including one in *Nature*) as well as meeting abstracts, presentations, and interactions. Also of note are continuing efforts toward the Coupled Model Intercomparison Project Phase 6 (CMIP6) activities, the Global Carbon Project Global Carbon Atlas (<http://www.globalcarbonatlas.org>), cooperative work with Chinese colleagues on better estimating their emissions, and press interactions.

LBNL Terrestrial Ecosystem Science SFA - Impact of warming on microbiology and carbon cycling in deep soils.

Eoin Brodie, Neslihan Tas, Caitlin Pries, Cristina Castanha and Margaret Torn (mstorn@lbl.gov)

Lawrence Berkeley National Laboratory

For the LBNL's Terrestrial Ecosystem Science SFA on soil carbon cycling, we are conducting research on the role of microbes in soil carbon turnover, storage, and loss—the impacts of climate change on these processes. We are focusing on deep soils because despite their low carbon density, subsoil horizons contain more than half of global soil organic carbon (out of 1,300–1,600 Pg organic carbon in the top meter). Moreover, the C turnover at depth is proposed to be slower than surface C, yet the vulnerability of deep soil carbon under future climate scenarios is yet to be understood. Microorganisms are responsible for both decomposition and formation of soil organic matter (SOM). The responses of microorganisms — changes in community composition, activity, gene expression, and physiology— determines how an environmental change will alter soil carbon and nutrient cycling. In this project, we aim to understand how long term warming impacts microbial community composition and decomposition of SOM in deep soils. To this end we established a soil warming experiment at the Blodgett Forest Research Station, located in the foothills of the Sierra Nevada, CA. The treatment warms the soil +4°C above ambient to >1 m depth while maintaining the natural temperature depth gradient. Samples across the soil profile were collected prior to the onset of warming and subsequently at six month intervals. Microbial community changes were analyzed via 16S rRNA gene sequencing and changes in microbial decomposition potential were assed via extracellular enzyme activity measurements of α - and β -glucosidase, cellobiohydrolase, N-acetyl- β -D-glucosaminidase and acid phosphatase. Additionally lab incubations with ^{13}C isotopologs of glucose and pyruvate were carried out to assess whether changes in microbial carbon use efficiency (CUE) occurred in response to warming. Although the activity of all enzymes declined with depth, we detected higher enzyme activities in response to heat treatment at each depth. Below the organic soil horizons, 20-60 cm showed the strongest enzyme activity response to the heating treatment. While microbial composition and diversity varied significantly through the soil profile, with increases in bacteria with oligotrophic growth strategies with depth. Over 18 month period however incubations with ^{13}C -labelled substrates demonstrated a 2-3 times increase in respiration due to warming. Metabolic modeling is being carried out to determine whether microbial CUE profiles correspond to microbial composition across the soil profile if CUE varies in response to warming.

ANL Terrestrial Ecosystem Science SFA:

CHARACTERIZING ORGANIC MATTER LABILITY IN ALASKAN TUNDRA SOILS USING MID-IR INFRARED SPECTROSCOPY

Zhaosheng Fan, Argonne National Laboratory, zfan@anl.gov

Roser Matamala, Argonne National Laboratory

Julie Jastrow, Argonne National Laboratory

Chao Liang, Argonne National Laboratory

Francisco Calderon, USDA-ARS

Gary Michaelson, University of Alaska Fairbanks

Chien-Lu Ping, University of Alaska Fairbanks

Umakant Mishra, Argonne National Laboratory

Scott Hofmann, Argonne National Laboratory

The permafrost region contains large amounts of soil organic carbon (SOC) that is preserved in a relatively un-decomposed state due to cold and often wet conditions, yet the potential lability of this SOC is still largely unknown. Traditional methods of assessing SOC lability (e.g., laboratory incubation studies) are labor intensive and time consuming. Fourier-transform mid-infrared spectroscopy (MidIR) provides a low-cost means to quickly estimate SOC quantity and quality based on the wealth of spectral information. The Argonne National Laboratory TES SFA explored the possibility of linking MidIR spectra with SOC lability in Arctic tundra soils. Soils from four sites on the North Slope of Alaska were used in this study: a low-centered polygon in the Coastal Plain (CP), a high-centered polygon in a lowland drainage area near Sagwon Hills (HC), a frost boil in an upland area near Sagwon Hills (SH), and a frost boil in an upland area near Happy Valley (HV). Active-layer organic and mineral soils and upper permafrost soils from the four sites were incubated for 60 days at -1, 1, 4, 8 and 16 °C. Incubated soils were allowed to drain to field capacity. Total SOC concentration and MidIR spectra of bulk soil samples were obtained before and after the incubations. Carbon dioxide (CO₂) production was measured throughout the incubations. SOC quality was independently characterized before incubation by quantifying several SOC fractions. We evaluated whether MidIR spectra could be calibrated by using multivariate partial least squares modeling to predict total SOC, CO₂ production, and the SOC fractions. Our results indicate that MidIR can be used to quickly and reliably estimate tundra SOC concentration and is a potentially power tool to quickly and reasonably estimate CO₂ production during short-term incubations. Future studies will determine whether this approach can be used to predict CO₂ production in longer term incubations designed to evaluate the intrinsic decomposability of permafrost-region soils. Our results also indicate that MidIR can be used to estimate measurable SOC fractions, which may be used to initialize, calibrate, and/or validate SOC pools of ecosystem and Earth system models.

Title: Peatland porewater chemistry responses to deep peat and whole-ecosystem warming

Authors: Natalie A. Griffiths¹ and Stephen D. Sebestyen²

¹Oak Ridge National Laboratory, Oak Ridge, TN, griffithsna@ornl.gov

²USDA Forest Service, Northern Research Station, Grand Rapids, MN, ssebestyen@fs.fed.us

Program: TES

Abstract:

SPRUCE is a 10-year long, whole-ecosystem experiment that is evaluating the response of a northern black spruce-*Sphagnum* bog ecosystem to elevated temperatures and CO₂ concentrations. A total of ten 12-m diameter enclosures were built in the S1 bog in northern Minnesota. Across the 10 enclosures, five temperature treatments (+0, +2.25, +4.5, +6.75, and +9°C) are replicated at ambient and elevated CO₂ concentrations (+500 ppm). Heating occurs both above and belowground, while CO₂ is added via the aboveground blower system. In June 2014, only belowground warming (deep peat heating; DPH) was initiated, providing the unique opportunity to evaluate the responses of deep peat soils to warming. In August 2015, whole-ecosystem warming (WEW) was achieved with the addition of aboveground warming. CO₂ addition is planned for summer 2016.

Within SPRUCE, we are collecting porewater samples weekly to biweekly along the peat profile (from 0 to 3 m into the peat) in order to understand how solute concentrations respond to warming and elevated CO₂. Porewater sampling was initiated in summer 2013, and we have characterized depth profiles for one year pre-treatment, throughout DPH, and for 4 months of WEW thus far. We predicted that total organic carbon (TOC) concentrations will increase with warming in both near surface and deeper porewaters due to mineralization of recently produced TOC and deep peat, respectively. We also predict that increased mineralization rates will increase dissolved nutrient concentrations. During DPH, there were no substantial changes in solute chemistry at depth (2 m), suggesting that deep peats are resilient to warming in the short term. During WEW, there was an increase in the magnitude and variability of TOC and potassium concentrations in near surface porewater (0 m) with increasing temperature. Porewater TOC concentrations almost doubled during WEW in the +9°C enclosures (mean concentration in each enclosure = 129, 121 mg/L) compared to the pre-treatment period (means = 64, 77 mg/L). Nutrient analysis on samples collected in 2015 is ongoing, and the response of nutrients to WEW will also be presented. pH, and other anions and cations examined did not change with WEW. These initial results suggest that carbon cycling responses to warming will likely be more dynamic in surface than in deeper peats. Overall, understanding the response of porewater chemistry to warming and elevated CO₂ is critical to interpreting changes in nutrient cycling, decomposition, and vegetation.

1 **Testing a land model in ecosystem functional space via a comparison of observed**
2 **and modeled ecosystem flux responses to precipitation regimes and associated**
3 **stresses in a central USA forest**

4

5 Lianhong Gu^{1*}, Stephen G. Pallardy², Bai Yang¹, Kevin P. Hosman², Jiafu Mao¹, Daniel
6 Ricciuto¹, Xiaoying Shi¹, Ying Sun³

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8 ¹Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National
9 Laboratory, Oak Ridge, Tennessee, USA

10 ²Department of Forestry, University of Missouri, Columbia, Missouri, USA

11 ³Jackson School of Geosciences, University of Texas, Austin, Texas, USA

12

13 *Corresponding author:

14 Lianhong Gu

15 Environmental Sciences Division, Building 4500N

16 Oak Ridge National Laboratory

17 Oak Ridge, TN 37831-6335.

18 Email: lianhong-gu@ornl.gov

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1 **Abstract**

2 Testing complex land surface models has often proceeded by asking the question: does
3 the model prediction agree with the observation? Such an approach has yet to produce a
4 solution to the ‘spaghetti problem of terrestrial models’. Here we test the Community
5 Land Model (CLM) by asking the question: does the model behave like an ecosystem?
6 We pursue its answer by testing CLM in the ecosystem functional space (EFS) at the
7 Missouri Ozark AmeriFlux (MOFLUX) forest site in the central USA, focusing on
8 carbon and water flux responses to precipitation regimes and associated stresses. In the
9 observed EFS, precipitation regimes and associated water and heat stresses controlled
10 seasonal and interannual variations of carbon uptake and water use in this deciduous
11 forest ecosystem. Such controls were exerted more strongly by precipitation variability
12 than by the total precipitation amount per se. A few simply constructed climate variability
13 indices captured these controls, suggesting a high degree of potential predictability.
14 While the interannual fluctuation in carbon uptake was large, a net carbon sink was
15 maintained even during an extreme drought year, suggesting a high degree of resilience
16 of this forest ecosystem to environmental stresses. Although CLM predicted seasonal and
17 interannual variations in evapotranspiration reasonably well, its predictions of carbon
18 uptake were too small across the observed range of climate variability. Also, the model
19 systematically underestimated the sensitivities of carbon uptake and evapotranspiration to
20 climate variability and overestimated the coupling between carbon and water fluxes.
21 Consequently, the modeled and observed trajectories of ecosystem fluxes did not overlap
22 in the EFS and the model did not behave like the ecosystem it attempted to simulate. We
23 suggest that future model improvements should focus on better representation and
24 parameterization of process responses to environmental stresses and on more complete

1 and robust representations of carbon-specific processes so that adequate responses to
2 climate variability and a proper degree of coupling between carbon and water exchanges
3 are captured.

4 **Key words:** Ecosystem Functional Space, Carbon and Water Budgets, Climate
5 Variability Indices, Land Surface Modeling, Eddy Covariance

6

**ORNL's Terrestrial Ecosystem Science – Scientific Focus Area (TES SFA)
A 2016 Overview**

Paul J. Hanson, Daniel M. Ricciuto and Project Participants
Climate Change Science Institute, Oak Ridge National Laboratory
Oak Ridge, Tennessee

Understanding responses of ecosystem carbon (C) cycles to climatic and atmospheric change is the aim of the Terrestrial Ecosystem Science Scientific Focus Area (TES SFA). Our vision is to:

Improved integrative understanding of terrestrial ecosystem processes to advance Earth System predictions through experiment-model-observation synergy

The TES SFA is guided by the vision that sensitivities, uncertainties and recognized weaknesses of Earth System Model (ESM) predictions inform observations, laboratory and field experiments and the development of ecosystem process modeling. In turn, predictive understanding and findings from the field and laboratory and improved process modeling are incorporated (with the associated uncertainties) into ESMs as explicitly and expeditiously as possible. Overarching science questions are:

- (1) How will atmospheric and climate change affect the structure and functioning of terrestrial ecosystems at scales from local to global and from decadal to centuries?
- (2) How will fossil fuel emissions and terrestrial ecosystem processes, mechanisms, interactions and feedbacks control the magnitude and rate of change of atmospheric CO₂ and other greenhouse gases?
- (3) What are the climate change-induced shifts in terrestrial hydrologic and ecosystem processes that inform assessment of climate change impacts on ecosystem services and society?

The proposed science includes large manipulations, C-Cycle observations, database compilation, and process studies integrated and iterated with modeling activities. The centerpiece of our climate change manipulations is the SPRUCE experiment testing multiple levels of warming at ambient and elevated CO₂ on the C feedbacks from a black spruce–*Sphagnum* ecosystem. **New efforts in 2016 include process studies of root traits and their potential to function to enhance or constrain biogeochemical cycles of ecosystems and their associated response to environmental change.** The TES SFA aims to integrate experimental and observational studies with model building, parameter estimation, and evaluation to yield reliable model projections. This integrated model-experiment approach fosters an enhanced, interactive, and mutually beneficial engagement between models and experiments to further our predictive understanding of the terrestrial biosphere.

Soil depths respond differently to *in situ* warming

Caitlin E. Hicks Pries, Cristina Castanha, Rachel C. Porras, and Margaret Torn

Lawrence Berkeley National Laboratory, Berkeley, CA, 94720, USA

Over half of global soil organic carbon (SOC) is stored in subsurface soils (>30 cm), but little is known about the vulnerability of this deep SOC to climate change. Most soil warming experiments have only warmed surface soils, so the temperature sensitivity of deeper SOC and its potential to generate a positive feedback to climate change is undetermined. We are currently investigating how SOC down to 1 m deep responds to experimental *in situ* soil warming (+4°C). Our field site is a coniferous forest in the foothills of the Sierra Nevada in California, USA. Our objectives are to understand (1) the dynamics of soil respiration at different depths, (2) how +4°C warming affects CO₂ production from different depths, and (3) how the temperature sensitivity of soil respiration differs by depth.

Warming began in October 2013, and we have successfully warmed 1 m of the soil profile to 4°C (±0.5) above ambient temperatures at each depth and maintained this warming throughout different seasons. We have taken monthly surface CO₂ flux measurements and monthly gas samples from stainless steel tubes at 15, 30, 50, 70, and 90 cm depths. We used Fick's law of diffusion and experimentally derived site-specific diffusion parameters to model CO₂ production from different depths. Warming significantly increased CO₂ production from all depths. Using the data from both treatments, we were able to estimate temperature sensitivity. Two indices of relative apparent temperature sensitivity (Q_{10} and E_a) indicate that the deeper soil is more temperature sensitive than the surface soil. However, no depths are sensitive to temperature at low soil moisture (VWC<0.25). Apparent temperature sensitivity is greatest during the winter, when soil moisture is high, which also suggests we are measuring a heterotrophic response. Despite the sensitivity of deep soil carbon to warming, only 11 to 13% of soil CO₂ production occurs below 30 cm even though 37% of all soil organic carbon is stored below 30 cm. The amount of carbon produced per gram soil is least in this deep soil implying deep soil C is overall less available to microbes overall. This study is one of the first to test whole-profile SOC responses to warming and shows that deep soil carbon is equally vulnerable to climate change in these upland mineral soils.

This work was conducted as part of the Berkeley Lab TES SFA.

ORNL's TES SFA Data Acquisition, Quality Assurance, and Archiving to Support Modeling and Synthesis Tasks

Les A. Hook*, Ranjeet Devarakonda*, Jeffery S. Riggs[^], Misha B. Krassovski*, W. Robert Nettles*, Paul J. Hanson*, and Thomas A. Boden*

*Environmental Sciences and [^]Logistical Services Divisions,
Oak Ridge National Laboratory

Data management, sharing, and archiving are an integral part of the ORNL TES SFA. The open sharing of all data and results from SFA research and modeling tasks among investigators, the broader scientific community, and the public is critical to advancing the mission of DOE's Program of Terrestrial Ecosystem Science. TES SFA researchers are developing and deploying the data systems, repositories, tools, and integration capabilities needed for the collection, QA, storage, processing, sharing, analysis, and archiving of data and model products.

These capabilities facilitate model-data integration and provide accessibility to model output and benchmark data for analysis, visualization, and synthesis activities in support of the TES SFA Vision. Active data sharing facilitates delivery of SFA products to sponsors, the scientific community, and the public. Task specific web sites, access to web-based tools, links to external products (e.g., microbial metagenomes), and data center value-added products (<http://tes-sfa.ornl.gov/>) enable these interactions.

The SPRUCE experiment (Spruce and Peatland Responses under Climatic and Environmental Change) is a key component of the SFA. SPRUCE has implemented an experimental platform for the long-term testing of the mechanisms controlling the vulnerability of organisms, ecosystems, and ecosystem functions to increases in temperature and exposure to elevated CO₂ treatments within the northern peatland high-carbon ecosystem. All data collected at the SPRUCE facility, all results of analyses or synthesis of information, and all model algorithms and codes developed in support of SPRUCE will be submitted to the SPRUCE Data Archive in a timely manner such that data will be available for use by SPRUCE researchers and, following publication, the public through the recently updated SPRUCE website (<http://mnspruce.ornl.gov>).

This poster highlights ORNL TES SFA tasks including data acquisition system development, data and modeling products, web-based tools, and their availability to project staff and the public.

Terrestrial Ecosystem Sciences program

Introducing FRED: A growing Fine-Root Ecology Database

Colleen M. Iversen^{1*}, A. Shafer Powell¹, M. Luke McCormack², Paul J. Hanson¹, Stan D. Wullschleger¹

¹Climate Change Science Institute and Environmental Sciences Division, Oak Ridge National Laboratory (ORNL)

²Department of Plant Biology, University of Minnesota

*E-mail: iversencm@ornl.gov

Variation and tradeoffs within and among plant traits are increasingly being harnessed by empiricists and modelers to predict ecosystem processes in response to current and future environmental conditions. While fine roots play an important role in ecosystem processes, most fine-root traits are extremely underrepresented in global trait databases. The lack of available and centralized data has hindered efforts to analyze fine-root trait variation at a global scale, and limited meaningful linkages among above- and belowground traits. Together, these limitations have contributed to the coarse representation of fine-root processes and associated parameters in terrestrial biosphere models. To address the need for a centralized fine-root trait database, we are compiling the Fine-Root Ecology Database (FRED) from published literature and datasets as well as unpublished sources; data collection is ongoing and will continue for the foreseeable future. To date, FRED contains ~39,000 species-specific trait observations from 936 species, and ~15,000 trait observations collected from mixed plant communities. In total, these observations encompass approximately 170 root traits. The observations housed in FRED are from ecosystems spanning the globe, but the data compiled thus far highlight in stark relief the *observations that are missing*. This is particularly striking for polar and boreal regions underlain by permafrost or characterized by organic soils, as well as tropical regions. In order to fill gaps in our global understanding and modeling of root traits and processes, we are focusing our belowground efforts in the SPRUCE (<http://mnspruce.ornl.gov/>) and NGEE Arctic (<http://ngee-arctic.ornl.gov/>) projects on quantifying the morphology, phenology, and depth distribution of fine roots, and linking these traits with ecosystem processes and environmental gradients.

FRED will be available to the broader community of modelers, root and rhizosphere ecologists, and applied ecological communities with unrestricted access through a website hosted by ORNL (roots.ornl.gov); we are targeting a release date of late 2016. We recognize that a considerable number of discrete trait datasets still reside with individual researchers, and we are actively encouraging the broader scientific community to contribute published past and future datasets to FRED. The website will serve as a location for the broader community to contact us and provide input or additional sources of data, and will also be used for communication and updates.

FRED is both global and growing, but more work is needed to improve our understanding of fine-root traits and their contribution to ecosystem processes, now and in the future.

ANL Terrestrial Ecosystem Science SFA:

Bioavailable Carbon and the Relative Degradation State of Organic Matter in Active Layer and Permafrost Soils

Julie Jastrow, Argonne National Laboratory, jdjastrow@anl.gov

Victoria Burke, Cardinal Stritch University

Timothy Vugteveen, Argonne National Laboratory

Zhaosheng Fan, Argonne National Laboratory

Scott Hofmann, Argonne National Laboratory

Jeremy Lederhouse, Argonne National Laboratory

Roser Matamala, Argonne National Laboratory

Gary Michaelson, University of Alaska Fairbanks

Umakant Mishra, Argonne National Laboratory

Chien-Lu Ping, University of Alaska Fairbanks

The decomposability of soil organic matter (SOM) in permafrost regions is a key uncertainty in efforts to predict carbon release from thawing permafrost. The cold and often wet environment is the dominant factor limiting decomposer activity, and SOM is often preserved in a relatively undecomposed or less humified state and can be poorly associated with soil minerals. Thus, the impacts of soil warming and permafrost thaw are likely to depend at least initially on the past history of SOM degradation before its stabilization in permafrost. The Argonne National Laboratory TES SFA is investigating the utility of soil fractionation approaches for assessing the relative degradation state of SOM and the amount of readily bioavailable soil organic carbon (SOC) in the active layer and upper permafrost of tundra soils in arctic Alaska. To assess the relative degradation state of SOM, we used particle size fractionation to isolate fibric (coarse) from more degraded (fine) particulate organic matter (POM) and separated mineral-associated organic matter into silt- and clay-sized fractions. To assess readily bioavailable SOC, we quantified salt (0.5 M K₂SO₄) extractable organic matter (SEOM), which correlates well with carbon mineralization rates in short-term soil incubations. In general, bulk SOC concentrations in permafrost were lower than in comparable active layers. Averaged across all soil layers, 60% of bulk SOC was found in POM. Even in mineral soils, about 40% of bulk SOC was in POM pools. Thus, overall, the organic matter in both active layer and permafrost soils was relatively undecomposed compared to typical temperate soils. In organic soils, SOM was more degraded in permafrost than in comparable active layers. But in mineral soils, this relationship was reversed; SOM was more degraded in the active layer than permafrost. For cryoturbated soils, the presence/absence of permafrost had no effect on degradation state. SEOM pool size was directly related to the quantity of POM carbon on a mass basis, but SEOM averaged only 1.2% of bulk SOC. However, the quality of the SEOM pool was more strongly related to the size of the organomineral pool (clay-sized fraction). Finally, analyses using this dataset showed that mid infrared spectra of bulk soils can be calibrated to predict the measured SOM fractions, which could facilitate widespread, high-throughput estimates of the size of the readily bioavailable carbon pool and organic matter degradation state for permafrost-region soils.

Functional Unit Testing in the Investigation of Black Spruce Foliar Dark Respiration

Anthony W. King^{*1}, Jeffery M. Warren¹, Daniel M. Ricciuto¹, and Anna M. Jensen²

¹ Climate Change Science Institute and Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge TN

² Department of Forestry and Wood Technology, Linnaeus University, Växjö, Sweden

*kingaw@ornl.gov

Understanding the temperature response of net photosynthesis, of both gross photosynthetic assimilation and foliar dark respiration (R_d), is needed in formulating informed hypotheses about vegetation response to temperature manipulations at the SPRUCE (Spruce and Peatland Responses Under Climatic and Environmental Change) site in northern Minnesota. Similarly, proper representation of temperature response is required of models like CLM-SPRUCE used to predict response to treatments and to extrapolate those responses spatially and into the future. It is generally quite difficult to interrogate fundamental processes such as leaf-level temperature response in integrated, fully coupled, operating earth system models, particularly under the controlled environmental conditions of field experiments. Site-specific models such as CLM-SPRUCE, with more flexible coding and shorter execution times, help in this regard but do not fully mitigate the issues. Thus the productive interplay between model and experiment is hampered. In response, we are using a functional testing framework to evaluate the functional representation of photosynthesis and R_d in CLM-SPRUCE and the land model of the Accelerated Climate Model for Energy (ACME). Here we report on results for pre-treatment (2010-2013) observations of the temperature response of R_d for black spruce (*Picea mariana*) at the SPRUCE site. In the functional unit testing framework, functional representations at the finest level of code granularity and the scale of observations are isolated as modular units. Results from these modules, under the controlled environmental conditions of experimental field (and laboratory) measurements, can be generated quickly and compared directly with experimental observations. Alternative formulations, observed and hypothesized, can be easily incorporated and evaluated. The framework also enables much easier data assimilation and sensitivity analysis at the level of functional units. Using this functional unit testing we have found that the observed temperature response of black spruce foliar R_d is not duplicated by the foliar R_d module of CLM-SPRUCE. The model simulates a reduction in $\ln R_d$ at temperatures > 30 °C not seen in the observations where $\ln R_d$ increases approximately linearly over the range 5-40 °C. The “acclimation” of R_d coded into the model may not appear in the observations because historically, black spruce at the site experience the warmer temperatures infrequently and only briefly. We use the functional unit testing to evaluate alternative representations of the R_d temperature response and discuss how insights obtained from the functional unit testing might inform hypotheses of black spruce R_d response to SPRUCE temperature treatments over the duration of the experiment.

Title: Microbial Response to the SPRUCE Deep Peat Heating Experiment

Authors: Laurel Kluber¹, J. Nicholas Hendershot¹, Samantha Allen¹, Daniel Yip¹, Zamin Yang¹, Paul Hanson², and Christopher Schadt¹

Author affiliations: ¹BioSciences Division and ²Environmental Sciences Division, Oak Ridge National Laboratory

Email: kluberla@ornl.gov, schadtcw@ornl.gov

Program: TES

Abstract:

The Spruce and Peatland Responses Under Climatic and Environmental Change (SPRUCE) experiment is a large-scale ecosystem manipulation designed to examine how peatland ecosystems respond to increased temperature and CO₂ levels. This experiment is expected to lead to various changes in ecosystem processes, including microbially mediated biogeochemical cycling, thus ultimately altering the overall C balance of these ecosystems. The initial phase of this experiment began over the summer of 2014 by heating deep subsurface peat to +2.25, +4.5, +6.75, and +9.0 °C above ambient plots with a target heating zone of 1.5-2 meters depth. Peat cores were collected in June 2014, September 2014 and June 2015, and microbial communities were examined at eleven discrete depths across the peat profile to a depth of 200 cm. One year of warming, microbial community structure and abundance of bacterial, archaeal, fungal, and methanogenic populations show strong vertical stratification across the peat depth profile yet no clear response to the temperature treatments. In an effort to identify factors that may be limiting decomposition and microbial community change, we conducted a microcosm incubation of deep peat (150-200 cm depth) at 6 and 15 °C to mimic ambient and +9 °C SPRUCE conditions. Additional treatments included elevated pH and the addition of N and P. Incubation microcosms were monitored for CO₂ and CH₄ production, and microbial community dynamics were assessed using qPCR and amplicon sequencing. Increasing temperature elevated both CO₂ and CH₄ production while elevated pH only resulted in greater CH₄ production. The effects of elevating temperature and pH in combination with N, P, or N+P additions were more variable. Although temperature had little effect on the overall microbial community structure, there was a shift in the size of bacterial and archaeal populations. In contrast, elevated pH and N additions seemed to have the largest influence on community structure and suggest that response in the deep peat may be limited by factors other than temperature.

A framework for the detection and attribution of terrestrial ecosystem dynamics

Jiafu Mao^{1†}, Whitney Forbes², Daniel M. Ricciuto¹, Mingzhou Jin², Xiaoying Shi¹, and Peter E. Thornton¹,

[1] Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN, USA

[2] Department of Industrial and Systems Engineering, University of Tennessee, Knoxville, TN, USA

The statistical methods of detection and attribution (D&A) have been widely used in studies of climate change and quantifications of causes underlying the multi-year changes. Their successful applications in the terrestrial ecosystems, however, are limited, mainly due to the lack of long-term and broad-scale observational records, and the lack of suitable simulations from both coupled and uncoupled models. We will overcome these challenges by proposing a framework that includes the development of effective D&A algorithms, the design of factorial land model ensemble simulations, and the assembling of observational and observation-based datasets at relevant scales. This work is expected to increase the efficiency and our confidence in attributing observed changes in carbon and water fluxes, and vegetation activities to extensive natural and anthropogenic factors.

ANL-Terrestrial Ecosystem Science SFA

Mid infrared spectral properties of northern soils across a latitudinal transect in Alaska

Roser Matamala, Argonne National Laboratory, matamala@anl.gov

Francisco Calderon, USDA-ARS

Julie Jastrow, Argonne National Laboratory

Chien-Lu Ping, University of Alaska Fairbanks

Gary Michaelson, University of Alaska Fairbanks

Zhaosheng Fan, Argonne National Laboratory

Umakant Mishra, Argonne National Laboratory

Scott Hofmann Argonne National Laboratory

We investigated the influence of site characteristics and soil properties on the chemical composition of organic matter in soils collected from a latitudinal transect across Alaska through analysis of diffuse reflectance infrared Fourier transform mid infrared (MidIR) spectra of bulk soils. The study included 119 soils collected from 28 sites including forest, tundra and grassland ecosystems. Organic, mineral, and cryoturbated soil layers from a variety of depths in the active layer and upper permafrost were included in the study. We found that organic matter chemistry as well as site and soil properties exerted a strong influence on the MidIR spectra. The spectra were very sensitive to the decomposition state of soil organic matter (SOM) as shown by MidIR differences among Oi, Oe and Oa organic layers. We found differences in peak intensity and area for several spectral bands when comparing Oi and Oa layers. The Oi layers had peaks at 3406, 2923-5, 2852-4, 1159-60 and 1052-60 cm^{-1} that were greater than Oa layers, suggesting that Oi layers contained greater abundance of labile residues and phenolic-OH compounds, aliphatic compounds (waxes, lipids and fats), and carbohydrates. In contrast, Oa layers had a greater presence of amide groups (possibly from microbial cells), aromatics, C=C bonds, carboxylates and carboxylic acids. Another significant factor differentiating the layers was the incorporation of clays and silicates into the decomposing organic matter of Oa layers. In addition, we found that MidIR spectra were related to many site/soil attributes including land cover type, parent material, and related factors, such as permafrost presence/absence, water permeability, soil depth, bulk density, cation exchange capacity, and pH. We identified specific bands that might be used in future studies to quickly estimate, from a single analysis, the total organic carbon (TOC), inorganic carbon, total nitrogen (TN), and TOC:TN of organic and mineral soils from Arctic and sub-Arctic regions. Our results show that the information contained in MidIR spectra

of bulk soil integrates SOM chemical composition with site environmental and soil conditions that influence SOM degradation state. The observed relationships also highlight the potential of linking information derived from MidIR to soil forming factors, which can facilitate geospatial extrapolations of SOM degradation state across the region.

Improving Soil C Dynamic Models Through the Incorporation of Microbial Processes

Melanie A. Mayes^{1,2}, Gangsheng Wang^{1,2}, Laurel A. Kluber^{1,3}, Christopher W. Schadt^{1,3}, and Wenjuan Huang^{4,5}

¹Climate Change Science Institute, Oak Ridge National Laboratory, ²Environmental Sciences Division, Oak Ridge National Laboratory, ³Biosciences Division, Oak Ridge National Laboratory, ⁴South China Botanical Garden, Chinese Academy of Sciences, ⁵Department of Ecology, Evolution, and Organismal Biology, Iowa State University

The focus of our research is to develop robust parameters and an improved conceptual understanding of microbial-facilitated decomposition of organic matter, and apply this knowledge to improve the Microbial ENzyme Decomposition (MEND) model. As part of this effort, we have been conducting a series of short to long-term (4 to 729 days) soil incubation experiments with ¹³C labeled glucose and cellulose, to examine how land use, edaphic properties, and microbial communities influence C use and the long-term fate of C in soils. Adjacent forested and grassland soils were collected from four sites including Alfisols in Missouri near the MOFLUX facility and another site in Athens OH, Ultisols in TN, and Mollisols from IA. Initial results show an expected trend of increased C mineralization and priming with glucose additions. However, long-term incubations indicate differential C use between forest and grassland soils, where cellulose addition had no effect on grassland respiration but suppressed C mineralization in forested soils. The results of these studies of longer-term soil C incubations will allow us to better parameterize MEND and other C cycle models with respect to the relationship between C source complexity and turnover rates in various soil types. In related studies, we are also incorporating soil moisture responses into the MEND model and testing the model against field-scale data from Ultisol soils at the Dinghushan Biosphere Reserve in China. We parameterized MEND using observed heterotrophic respiration (R_H) and microbial biomass C (MBC) from a three-year field experiment in two subtropical forests: a young pine forest (PF) and an old-growth broadleaf forest (BF). The observed seasonal variability in both MBC and R_H were well fitted by the MEND model. Both MBC and R_H in the two forests were more sensitive to soil moisture than to temperature, and the R_H in BF was more susceptible to soil moisture than that in PF. The R_H increased to a larger extent in the wet season, potentially by inducing a greater active fraction of microbial biomass in BF than PF. Our results suggest that the microbial controls on soil C decomposition are different with forest types. The soil microbial community tends to decrease in abundance under a drought-prone environment in BF, and MEND simulations suggest that this effect would enhance soil C storage. Together these studies are further elucidating the factors influencing the fate of soil C and will allow us to further refine the efficacy and environmental sensitivity of the MEND model.

Synthetic Mineral-Organo Associations in Soil: Vulnerability of Mineral Associated Carbon to Microbial Decomposition with Depth

Rachel C. Porras, Peter S. Nico, Caitlin Hicks Pries, and Margaret Torn
Lawrence Berkeley National Laboratory, Berkeley, CA, 94720, USA

Rachel C Porras, Lawrence Berkeley National Laboratory, Berkeley, CA, United States

Globally, soils, including deeper subsoils (>30 cm), represent an important reservoir of soil organic carbon (SOC) that can potentially be of great importance to the carbon cycle. However, the bioavailability of this SOC and, in particular mineral-associated SOC, to microbial decomposer communities and its potential to amplify the effects of climate change is highly uncertain. To gain insight into the bio-accessibility of mineral-associated organic C, we conducted a series of incubations using soils collected from three depths (0-10, 50-60, and 80-90 cm) under coniferous forest. The soils are moderately acidic (~pH 6.5) sandy, mixed, mesic Ultic Haploxeralfs.

To understand how mechanisms controlling SOC bio-accessibility differ with depth and with the properties of mineral-organo associations (MOAs), we synthesized two common soil minerals, goethite and ferrihydrite. ^{13}C labeled MOAs were prepared by reacting the synthetic Fe oxides with 9.9 atom % ^{13}C labeled glucose for 12h in the dark. Synthetic MOA's were initially created at 100% of maximum sorption capacity and gently washed to remove non-absorbed and weakly held interstitial material. Post washing, goethite MOAs retained 52% of added glucose while ferrihydrite MOAs retained 77%. The synthetic MOAs were added to aliquots of soil collected from each of the three depths. The soils containing the ^{13}C labeled mineral-organo associations were incubated at 20°C.

Respired $^{13}\text{CO}_2$ was measured and used to estimate the amount of microbially decomposed mineral associated ^{13}C -glucose. After 72 hours, 92% \pm 3%, 36% \pm 3%, and 26% \pm 3% of ^{13}C labeled glucose added directly to soils in our controls was decomposed for 10-20cm, 50-60cm, and 80-90cm, depth increments respectively, indicating generally high availability of the fresh glucose. In contrast, less than 0.2% of mineral associated ^{13}C -glucose was decomposed for either of the synthetic MOAs confirming that association with reactive mineral surfaces does dramatically retard microbial decomposition of otherwise readily biodegradable organic substrates in soils. Calculated $^{13}\text{CO}_2$ flux rates were similar for synthetic goethite- and ferrihydrite-organo complexes and also showed a decrease with depth. Interestingly, a 'disturbance control,' in which glucose free ferrihydrite was added to the soils, resulted in an apparent slight decrease in baseline respiration. This effect decreased with depth, and if confirmed could indicate a potential impact on carbon availability of unsatisfied mineral surface area at depth.

This work contributes to the Lawrence Berkeley National Laboratory Terrestrial Ecosystems Sciences SFA.

A new model intercomparison at SPRUCE

Daniel M. Ricciuto^{1,*}, Xiaoying Shi¹, Leslie A. Hook¹, Bai Yang¹, Jiafu Mao¹, Jitendra Kumar¹, Xiaofeng Xu², Paul J. Hanson¹

¹ Environmental Sciences Division and Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA

² Department of Biology, San Diego State University, San Diego, CA, USA

*Author to whom correspondence should be addressed; E-Mail: ricciutodm@ornl.gov; Tel.: +1-865-574-7067; Fax: +1-865-574-9501.

Quantifying the impacts of climate change on and potential feedbacks from carbon-rich peatland systems is critically important to Earth system predictions. To improve understanding of peatland processes, a whole-ecosystem warming experiment began at the Spruce and Peatlands Responses Under Climatic and Environmental Change (SPRUCE) site in northern Minnesota in 2015, and addition of atmospheric carbon dioxide is beginning in 2016. Initial *a priori* simulations from a small number of models indicated widely varying carbon dioxide and methane flux responses to warming and CO₂ addition depending on the model assumptions. A more formal model intercomparison is now underway to evaluate model predictions of pre-treatment conditions and to form hypotheses about decadal-scale effects of the manipulations. Participating modelers are providing detailed information about model structure and parameters that will help us better understand the sources of prediction uncertainty. Historical meteorological and environmental pre-treatment driver datasets have been provided and initial simulations using these forcings are shown. Plot-level driver datasets with specific temperature and CO₂ manipulations, including chamber effects (e.g. on snowfall, and solar radiation), are being constructed to represent several possible future scenarios over the course of the experiment. These scenarios will be used to assess the impact of interannual variations in climate superimposed on the treatments, for example consecutive drought or wet years. Models will also be provided with century-scale climate change scenarios to predict the peatland responses over long timescales.

Representing northern peatland hydrology and biogeochemistry with the Community Land Model

Xiaoying Shi¹, Daniel M. Ricciuto¹, Peter E. Thornton¹, Paul J. Hanson¹, Xiaofeng Xu², Jiafu Mao¹, Steve Sebestyen³, Jeffrey Warren¹, Richard J. Norby¹, and Natalie A. Griffiths¹

¹Climate Change Science Institute /Environmental Science Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

²Biology Department San Diego State University, San Diego, CA, 92182-4614, USA

³USDA Forest Service Grand Rapids, Minnesota

Northern peatlands are likely to be important in future carbon cycle-climate feedbacks due to their large carbon pool and vulnerability to hydrological change. Predictive understanding of northern peatland hydrology is a necessary precursor to understanding the fate of massive carbon stores in these systems under the influence of present and future climate change. Current models have begun to address microtopographic controls on peatland hydrology, but none have included a prognostic calculation of peatland water table depth for a vegetated wetland, independent of prescribed regional water tables. We introduce here a new configuration of the Community Land Model (CLM) which includes a fully prognostic water table calculation for a vegetated peatland. We also couple our new hydrology treatment with vertically structured soil organic matter pool, and the addition of components from methane biogeochemistry. We inform and test our model based on SPRUCE experiment to get the reasonable results for the seasonal dynamics water table depths, and correct soil carbon profiles. Then, we use our new model structure to test the how the water table depth and CH₄ emission will respond to elevated CO₂ and different warming scenarios. Finally, we will test the modeling contrasting responses of the peatland carbon exchange both CO₂ and CH₄ with atmosphere to changes in water table depth.

Abstract

MS Torn, Caitlin Hicks Pries, Rose Abramoff, Katerina Georgiou, Rachel C. Porras, Cristina Castanha, Eoin Brodie, Neslihan Tas, Peter Nico, Bill J. Riley.

Title: Berkeley Lab Terrestrial Ecosystem Science SFA: Belowground carbon cycling

In the Berkeley Lab Terrestrial Ecosystem Science SFA, we conduct basic research on the role of soils in terrestrial biogeochemistry and climate feedbacks. Our goals are to improve process-level understanding of ecosystem-climate interactions and to develop next-generation predictive capacity suitable for Earth System Models. Current research in the SFA is centered around a coordinated set of model, field, and laboratory experiments to quantify and characterize the relative roles of different soil organic-matter stabilization and destabilization processes and soil-plant-microbe-nutrient interactions, and how they may shape ecosystem responses to climate change. We are using field manipulations of soil temperature across the soil profile to evaluate the influence of soil depth and mineralogy, soil biota, and soil microclimate on soil carbon dynamics, and applying these research results and observations to develop and test new model structures and parameters. In this phase of the SFA, we aim to improve process-level understanding of the controls of soil carbon turnover and stocks and develop the belowground component of ESMs and fine scale models. This poster will present three whole-profile soil warming experiments, in a grassland, a coniferous forests, and an Arctic tundra ecosystem (the latter research is part of the DOE NGEE Arctic project) and give an overview of microbial, mineralogical, biogeochemical, and modeling work being carried out in the SFA. More detail is given in separate posters on each of those four areas.

Global sensitivity analysis of a leaf photosynthesis model composed of multiple competing hypotheses

Anthony Walker, Ming Ye, Heng Dai, Martin De Kauwe, Dan Lu, Dan Ricciuto

Accurate quantification of model sensitivities and uncertainties informs rigorous model inter-comparison, experiments targeted to improve models and maximise uncertainty reduction, and probabilistic forecasts for risk based planning in the face of future environmental change. Until now, comprehensive global methods have been available to assess model sensitivity only to variation in parameters but not to variation in the representation of processes. Systems models combine many sub-systems and processes, each of which may be conceptualised and represented mathematically in various ways. The sensitivity analysis method demonstrated here quantifies the variability in a model outcome caused by variability in process representation.

Plant photosynthetic rates increase in response to elevated atmospheric CO₂, increasing plant carbon availability. These physiological responses to CO₂ are well understood yet the response of the terrestrial carbon sink to increasing atmospheric CO₂ remains the largest uncertainty in global C cycle modelling to date. There are many sources of this uncertainty. We hypothesise that a portion of this uncertainty is related to the different assumptions that can be made while modeling photosynthesis. In this study we take an initial step towards formally assessing the sensitivity of the modelled leaf carbon assimilation response to CO₂ caused by multiple incarnations of the Farquhar model and variable parameters. Results are for demonstrative purposes only as the method is under active development for improved computational efficiency. We hope this work will provide an extremely useful and rigorous framework for the process of model development, comparison, and selection.

Building A Virtual Ecosystem Dynamic Model for Root Research

Y. XU, D. Wang, C. Iversen, A. Walker, J. Warren

Understanding the fundamental mechanistic processes within large environmental models has great implications in model interpretation and future improvement. However, obtaining a good understanding of these processes can be challenging due to the complexities in model structures and software configurations. This effort uses a function test framework – with unique approaches to tackling software complexities in large environmental models – to facilitate process-based model exploration and validation. A Virtual Ecosystem Dynamic Model is developed as a case study to better understand and validate root-related processes in the ACME Land Model (ALM). The proposed framework could help empiricists better access the inner workings of large environmental models, and facilitate integrative collaborations among broad scientific communities including field scientists, environmental system modelers, and computer scientists.

Ecophysiology and water relations of woody plants within an *Picea-Sphagnum* ombrotrophic bog

Jeffrey M Warren, Anna M Jensen, Stan D Wullschleger, Paul J Hanson
Oak Ridge National Laboratory, Oak Ridge, TN, 37831

Beginning in 2015, the Spruce and Peatland Responses under Climatic and Environmental Change (SPRUCE) climate change experiment (<http://mnspruce.ornl.gov/>) in Northern Minnesota, USA, will expose 13 m diameter plots of an ombrotrophic *Picea mariana* – *Ericaceous* shrub – *Sphagnum* bog ecosystem to long-term temperature × CO₂ treatments. Treatments are expected to change soil water availability, vapor pressure deficit, photosynthesis, respiration, evapotranspiration and relative species composition. We examined pre-treatment ecophysiology of *Picea mariana* (black spruce) including seasonal assessment of cohort specific light-saturated assimilation rate (A_{max}), maximum electron transport rate (J_{max}), maximum carboxylation capacity (V_{cmax}), respiration and their temperature response functions. In addition, we assessed diurnal and seasonal patterns of sap flow and species-specific patterns of water potential. Granier-style thermal dissipation probes (TDP) were calibrated *in situ* by cutting instrumented trees and measuring their actual water uptake. We also assessed spruce hydraulic conductivity under drying conditions in excised roots, branches and foliage using vulnerability curves and pressure-volume curves.

Photosynthetic capacity increased as the season progressed, and peaked by late summer, with the 1-2-year-old cohorts contributing more than new needles to modeled total C uptake. V_{cmax} and J_{max} were not responsive to T in the spring, however, by August they were highly sensitive to T, with optimal T peaking between 35-38°C, slightly higher than current maximum summer air T. The SPRUCE experimental treatments will push air T up towards 45°C in some plots, which will allow us to test foliar capacity for biochemical T acclimation. Sap flow began by late May and was fairly constant over the season until declining in mid-September and ceasing as temperatures dropped below zero. The *in situ* calibrations improved sap flow estimates, and illustrated substantial hysteresis in sap flow due to release of stored water in larger trees. Midday mean summer ψ was -1.5 MPa for spruce foliage, higher than the co-occurring *Larix laricina* (larch), which was -2.0 MPa. Laboratory measurements indicated specific leaf conductivity of spruce declined as drought stress increased beyond -1.2 MPa, with the average turgor loss point (TLP) reached by -2.5 MPa, lower than the TLP of larch (-1.95 MPa). While summer spruce ψ remained higher than the TLP, larch often reached the TLP indicating substantial loss of hydraulic conductivity on a daily basis, indicating potential for shifts in community composition due to treatment effects on net carbon uptake and differential water stress among the species.

Insights into *Sphagnum* physiology and the associated microbiome at SPRUCE

David J. Weston, Alyssa Carrell, Richard J. Norby, Joanne Childs, Anthony Walker, Jana Phillips, Paul Hanson

Climate Change Science Institute, Oak Ridge National Laboratory, Oak Ridge, TN

The SPRUCE experiment is a large-scale peatland manipulation with multiple levels of warming at ambient or elevated CO₂ in a *Picea mariana*–*Sphagnum* peat bog in northern Minnesota. *Sphagnum* species are a dominant component of the SPRUCE community profile and boreal peatlands in general. At the SPRUCE site, The *Sphagnum* dominated moss layer is estimated to contribute to approximately 47 – 49% of net primary production (NPP) and is considered a critical component for maintaining low bog pH and N inputs through its associated microbiome. We installed eight clear-top automated gas exchange chambers (Li-COR 8100s) in hollows to assess *Sphagnum* net ecosystem exchange of C (NEE). Daily integrated values of chambers showed a slight trend in net CO₂ uptake in the beginning of the season that quickly transitions to a peak in CO₂ release during the middle of the season and gradually increases to near neutral or compensation values from September to November. Both gross primary productivity and peat/*Sphagnum* respiration peaked in mid-August and followed a near asymmetric distribution with the time from spring thaw to peak values. Insight from modeling activities suggests that considerable nitrogen (N) must be fixed and transferred to *Sphagnum* plants to support the observed production rates. To gain insight into the composition of the *Sphagnum* associated microbiome and possible role in N fixation, 16S rRNA profiling was performed within the experimental enclosures of the warming treatments. We found all samples to be dominated by *Alphaproteobacteria* (45-51%) followed by *Acidobacteria* (11-16%) and *Gammaproteobacteria* (8-9%). The functional member abundance varied by warming treatment: diazotroph abundance decreased with increased temperature (6% in ambient control, 3% in ambient +6C) while methanotroph abundance increased with temperature (0.14% in ambient control, 1.3% in ambient +6C respectively). The consequence of this functional community member shift is not clear and merits further exploration. A current collaboration with the DOE Joint Genome Institute has now expanded the genomic resources for this project by providing two draft genomes for *S. fallax* and *S. magellanicum* and the resequencing of a 200 individual *S. fallax* pedigree. Together with isolated fungal and bacterial strains, this represents a tremendous resource to the biological community interested in plant – microbe interactions, evolutionary and ecological genomics, and peatland ecology.

Improve the representation of phosphorus availability and uptake in land surface models

Xiaojuan Yang, Peter Thornton, Dan Ricciuto, Richard Norby, and Forrest Hoffman
Oak Ridge National Lab, Oak Ridge, TN 37830

Phosphorus (P) has been shown to limit a number of fundamental ecosystem processes and is considered the nutrient most limiting to carbon cycling in lowland tropical forests. Despite the importance of P in terrestrial ecosystems, none of the models in the IPCC AR5 considered P as a limiting nutrient, and the modeling community only recently started to implement P dynamics and carbon-nitrogen-P interactions into land surface models (e.g. CASA-CNP, JSBACH-CNP and ACME-CNP). Still, some key processes controlling P availability and P uptake are either not well represented or not considered due to limited understanding and lack of readily available data. Here we try to improve the representation of soil P availability and uptake in ACME-CNP by introducing the effects of soil pH and root exudates on soil P dynamics. We also investigate how different representations of phosphatase biochemical mineralization affect simulated soil P availability.