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PNNL-30628

Biogeochemical Processes Across Aquatic Interfaces

October 2020

Jianqiu Zheng

U.S. DEPARTMENT OF ENERGY

Prepared for the U.S. Department of Energy
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Report

Project Summary The aquatic interfaces exposing terrestrial soils to oxic-anoxic regime shifts represent biogeochemical “hotspots” that are extremely sensitive to climate and environmental change. However, processes and interaction across theses aquatic interfaces are poorly understood and underrepresented in current Earth system models. In this project, we aim to develop predictive understanding of the feedbacks between microbial systems and geochemical environments that determine emergent ecosystem behaviors and resilience in response to disturbances. We use experimental, mechanistic modeling and meta-analysis tools to elucidate interactions among soil, water, geomorphology and microbiology that regulate the molecular transformations and fluxes of carbon, nutrients, and redox sensitive compounds across aquatic interfaces.

Introduction and Project Description

The aquatic-terrestrial interfaces within and between ecosystems are biologically and geochemically active components of the Earth system featuring steep physical, chemical and biological gradients and rapid biogeochemical transformations. Multiple drivers interact to control ecosystem outcomes, impeding our ability to accurately predict ecosystem response to climate and environmental changes using traditional terrestrial or aquatic models that solely focusing on organic matter (OM) stability or water residence time and transport, respectively. We developed an integrated modeling framework incorporating strengths from both terrestrial- and aquatic- originated modeling concepts to gain predictive understanding of the coupled OM decomposition and redox reactions under the impact of dynamic geochemical environmental conditions. To understanding the relative importance of environmental geochemical constraints and microbial functional traits in regulating biogeochemical transformations, we designed a data synthesis study examining microbial community compositional and function shifts along environmental gradients, together with a laboratory incubation study elucidating the influence of redox levels and salinity gradient on soil redox reactions and greenhouse gas productions, we could complete our model-data integration loop for developing predictive understanding of biogeochemical cycling across aquatic interfaces.

Results and Accomplishments

<u>Modeling:</u> We built a new modeling framework simulating processes and interactions among OM, microbes, and minerals. Within this new framework, we established substrate explicit configuration to represent the varying reactivity of OM substrates and further incorporated pathway-specific microbial energetics to represent microbial functional and physiological traits. This work leads to two manuscripts: **Adapting carbon dynamic models to characterize biogeochemical processes across aquatic interfaces (PNNL-SA-156498)** and **Thermodynamic and kinetic constraints on microbial mediated redox biogeochemistry**.

<u>Meta-analysis:</u> We conducted a meta-analysis on microbial community shift along salinity gradient to inform trait-based microbial model development. This work is summarized in manuscript **Meta-analysis reveals consistent microbial community response to salinity gradient (PNNL-SA-156653)**. Ad a follow-up of this analysis, we conducted an additional meta-analysis aiming to gain insights on the contributions of microbial functional redundancy in regulating microbial mediated element cycling. This work leads to a manuscript **Redundancy of microbial functions associated with elemental cycling across the globe (PNNL-SA-155318)**.

Experiments: We conducted series of microcosm experiments investigating the transition of electron accepting processes in response to redox and salinity gradients. We generated time series data of carbon fluxes and aqueous phase chemistry that were used for model calibration. However, we were not able to complete the 16S-based microbial community analysis and qPCR-based quantification of microbial functional groups due to the impact of pandemic.

Software: We developed an R package with model inner-comparison and optimization capabilities to address computational challenges in model selection and model-data fitting. This work has been partially complected, and we're in the process of manuscript development for package release. A test version of this R package can be accesses at https://github.com/jianqiuz/MENDplus.

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