Biogeochemical Consequences of DOM Chemistry, Microbial Gene Expression, and Nutrient Concentrations: Integration between Lab Experiments and Substrate/Microbially-Explicit Models Linked to Reactive Transport

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This element of the PNNL SFA seeks to understand biogeochemical consequences of variation in DOM chemistry, microbial gene expression, and nutrient concentrations, and integrate that knowledge with a modeling framework that couples these features with reaction network and reactive transport models. Here we will experimentally evaluate the biogeochemical consequences of variation in DOM chemistry, microbial gene expression, and nutrient concentrations. We will extend analyses beyond net respiration rates to data/insights needed for reaction network models that couple DOM with nutrient cycles. Previously the SFA has used high resolution DOM characterization, nutrient concentrations, and respiration rates to reveal that aerobic respiration undergoes a metabolic paradigm shift from DOM thermodynamic regulation under C-limitation to N-mining regulation under C-replete environments. The functional forms and cross-system generality of such relationships remain unknown, however.
These knowledge gaps limit our ability to represent basin-scale spatial and temporal changes in mechanisms linking DOM chemistry, microbial gene expression, and nutrient concentrations to river corridor hydrobiogeochemical function.

We will use a combination of laboratory experiments (batch reactors) and reaction network modeling to resolve knowledge gaps and provide a process-based modeling framework. Lab experiments will use sediments from reaches with maximum contributions from sediment to river corridor respiration in each of four sub-basins across the Columbia River Basin (CRB).
Sites will span CRB functional zones to evaluate transferability of experimental outcomes and associated models. DOM concentration and the presence of organic N will be manipulated, followed by measurements of respiration, nutrients (e.g., NH_4^+, NO_3^-, Fe(II), N_2O), DOM molecular properties (FTICR-MS, GC-MS, LC-MS, NMR), and microbial metatranscriptomes.

Data spanning DOM chemistry, gene expression, and nutrient concentrations will be used with a cheminformatics/metabolic modeling pipeline linking molecular information to 1D PFLOTRAN in KBase. A critical component is leveraging multi-omic data to identify biogeochemical reaction networks for reactive transport modeling in PFLOTRAN. Models will be run independently in each sampled field location. Simulated dynamics of DOM chemistry, gene expression, and solute transformations will be studied using machine learning and other data-driven modeling techniques to discover simplified representations of the linkages among molecular properties/processes and nutrient dynamics across environmental conditions. This will provide a foundation for reduced-order basin-scale models that link molecular properties/processes to basin-scale hydrobiogeochemical dynamics.