Integrated Modeling of Carbon and Nitrogen Cycling in River Corridors Across the Yakima River Basin

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Project Abstract: *This element of the PNNL SFA seeks to quantify the cumulative impacts of river corridor hydrologic exchange flows (HEFs), dissolved organic matter (DOM) chemistry, and microbial activity on biogeochemical cycling, water quality, and contaminant mobility across the Yakima River Basin (YRB) under both baseline and disturbance conditions.* River corridors play important roles in carbon and nitrogen cycling and removal of excess nutrients. We are developing a new approach to mechanistically represent the river corridor as an integral part of a watershed using unstructured meshing in ATS, seamlessly linking dynamic river flow processes and heterogeneous terrestrial inputs. Leveraging ATS-PFLOTRAN coupled through the Alquimia interface from the IDEAS-Watersheds software ecosystem, we performed coupled hydrologic and biogeochemical modeling at the American River watershed to investigate water, energy, and solute fluxes across the river-groundwater interface in connection to variations in land use, hydrogeology, climate, and disturbances. The biogeochemical hot spots and hot moments within the river corridors are found to be strongly influenced by riverbed properties and flow conditions. SWAT models are set up across the Yakima River Basin (YRB) to study how watersheds respond to wildfires of various burn severity and history. The simulated water quantity and water quality responses (e.g., water temperature, suspended solids, total nitrogen and total phosphorous) are used to guide where we perform sampling and monitoring within the YRB to improve the predictive understanding of fire impact. Machine learning methods have been applied to integrate data from USGS river gauges and remote sensing to improve model parameterization and calibration. By exploring interactions among these three watershed response variables, i.e., streamflow, evapotranspiration and snow cover, for calibrating the ATS model at the American River Watershed, we found that remotely sensed ET data products might provide as useful information as the streamflow for watershed model calibration in cases where stream gage data are unavailable. Our approach can be generalized beyond the YRB and applied to other basins facing environmental disturbances and water challenges of national significance.

Hydrobiogeochemical Variability: Mechanisms Governing Reaction- to Basin-Scale Hydrobiogeochemical Regimes

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Project Abstract: *This element of the PNNL River Corridor SFA seeks to identify places/times across the Yakima River Basin (YRB) in which sediment-associated metabolism strongly influences active channel biogeochemistry, and to reveal drivers of underlying molecular properties.* To represent processes governing river corridor biogeochemistry in predictive models, we need to understand how and why biogeochemical contributions from sediment-associated organisms vary through space/time; such contributions vary from 3-96% of respiration. Recent RCSFA work predicts spatial variation in sediment contributions to respiration. To evaluate these predictions, we are deploying sensor systems across 2nd-7th order streams in the YRB. Site locations were selected using a multi-iteration ModEx approach. Sites span four sub-basins in the YRB and are distributed across multiple complementary efforts that each focus on time series (discussed here) or spatial variation (discussed in a separate presentation). The temporal component includes 6 sites distributed across stream orders and biomes from low order mountain settings to high order lowland rivers adjacent to agricultural and urban areas, coinciding with other agencies' gauging installations. The 6 sites have been visited every 1-2 weeks starting in April 2021 to collect *in-situ* measurements and water samples for standard measurements (e.g., organic C concentration, ion chemistry, carbonate/bicarbonate speciation) and less standard measurements (e.g., FTICR mass spectrometry), to provide model-relevant data. Initial analysis of the FTICR data indicates that many organic matter characteristics vary with catchment area. Specifically, both organic matter functional diversity, as it relates to biodegradability, and the potential for varied biogeochemical organic matter transformations increased with increasing catchment area. Starting in November 2021, preliminary deployments of automated dark-bottle incubation systems (autochambers) were initiated. These autochambers are designed to estimate the fraction of system respiration from sediments by measuring the difference between water column and ecosystem respiration rates in the river corridor. These are novel sensor systems, and the initial deployments are designed to generate time-series data and test/improve system function and reliability prior to larger-scale deployments. Data reduction and QA/QC has been developed and employed to generate sensor-based datasets. Lab analysis of samples is completed as samples are generated, and QA/QC is ongoing. These sensor- and sample-based time series will be used to drive and evaluate reaction networks in the dynamic basin-scale models used by the RCSFA.

The Influence of Wildfire Disturbance on River Corridor Hydrobiogeochemical Function

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Project Abstract: *This element of the RCSFA aims to reveal the mechanisms by which wildfires influence biogeochemical cycling in river corridors from reaction to basin scale. Our objective is to improve model predictive capacity in watersheds impacted by fire disturbances, important for ascertaining the influence of fire on ecosystem structure and function*. Wildfires generate a spectrum of physical and chemical alterations to terrestrial vegetation (i.e., char and ash), which alter runoff materials entering inland waters; these altered materials and pathways can change aquatic ecosystem functions. Recent thermodynamic modeling work supports emerging theories that pyrogenic organic matter (PyOM) – a portion of these materials – is more bioavailable than traditionally accepted, supporting growing evidence that it may be an underappreciated driver of river corridor biogeochemistry. Most research on changes in char chemistry focuses on the continuum of combustion temperatures created in the laboratory and does not target shifts in burn severities seen in the landscape. Therefore, we designed and implemented an open-air burn table experiment to investigate how chemistry of vegetation-derived chars and their leachates changes with burn severity metrics. Initial experiment results showed organic phosphorus (P) was increasingly converted to calcium-associated inorganic P forms in chars with higher burn severity, while total percent carbon (C) and nitrogen (N) increased from parent feedstock to low severity burns, then subsequently decreased with increasing burn severity. We found higher severity burns had lower concentrations of dissolved C and N than lower severity burns, and shrubland feedstocks were more soluble than conifer feedstocks. These contrasting changes to organic matter (OM) and inorganic nutrient composition indicate that wildfires in different ecosystems may uniquely impact downstream riverine biogeochemical processes across common wildfire fuel types. Differences in OM chemistry at the landscape scale are also being examined through high resolution storm sampling across 5 western Oregon watersheds in the Holiday Farm Fire burn perimeter. We find that post-fire storms elevated the transport of surface materials to streams within the burn perimeter in which the quality of material delivered was controlled primarily by burn severity within the catchment. Additionally monthly changes in OM chemistry are being investigated in a semi-arid sub-watershed of the Yakima River Basin. We are modeling and monitoring in- and out-of-fire impacted stream reaches in the context of shifting C:N:P dynamics to assess the influence of fires on the relationships between C, N, and P cycling.

Hydrobiogeochemical Features and Function Across Basins

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Project Abstract: *This element of the PNNL River Corridor SFA combines molecular data and numerical modeling to provide transferable principles that integrate organic matter (OM) chemistry and microbial gene expression.* We extend the RCSFA to the globe using crowdsourcing to further establish ESS as a global leader in open watershed science. We are leveraging WHONDRS data while shifting the sampling paradigm to efforts guided more directly by models, via deeper stakeholder engagement, and in partnership with other ESS investments and other agencies (e.g., USDA, NSF, DoD). For example, we are using AI models to guide new sampling locations (see ICON-ModEx presentation) and partnered with EXCHANGE and the University of Quebec to study OM chemistry from source to sea along the St. Lawrence River. We are also expanding to additional continents such as Africa and South America. From each of these sampling efforts, we also generate metagenomic and metatranscriptomic data with JGI. These data are being integrated into the Genome Resolved Open Watersheds database (GROWdb). GROWdb goes beyond the RCSFA and provides an open resource for global river corridor microbiomes. To date, 360 river microbiomes have been sampled across the globe and ongoing sampling aimed at filling in geographical gaps. Microbiomes from all sites were characterized using genome resolved metagenomics, enabling the reconstruction of thousands of unique microbial genomes and a corresponding catalog of over 2 million microbial genes, including sampling of 850 genes with known capacity to modulate carbon, nitrogen, sulfur, and hydrogen cycling in these watersheds. GROWdb has partnered with DOE KBase to make this resource publicly available and to enable integration of river-specific microbial processes into reactive transport models through genome-scale metabolic models, with 2,093 models built to date. Approximately a third of the samples have paired metatranscriptomes and metabolomes, distinguishing active from latent microbial processes and providing additional constraints for modeling efforts.

Mechanisms Governing Spatial Variability in River Corridor Hydrobiogeochemistry

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Project Abstract: *This element of the PNNL River Corridor SFA seeks to understand spatial variability in hydrobiogeochemistry across the Yakima River Basin (YRB).* To represent processes governing river corridor hydrobiogeochemistry in models, we need to understand hydrobiogeochemistry across broad environmental gradients that include natural (e.g., fire) and anthropogenic (e.g., urban) disturbances. To help fill this need we are studying spatial variation in river corridor chemistry, microbiology, and aerobic respiration across 47 sites in the YRB. Sites were selected using an iterative ModEx approach. Integrated teams selected model-relevant variables for both standard (e.g., dissolved organic C concentration, major ion chemistry) and less standard measurements (e.g., organic matter chemistry via FTICR). Numerical simulations were coupled with AI methods to identify system features most strongly associated with predicted variation in river corridor hydrobiogeochemistry. These key features were used to cluster YRB rivers into classes. Field sites were selected across all classes while accounting for logistical constraints of field work. Resulting sites were distributed across stream orders, biomes, and land cover/land use from low order mountain settings to high order lowlands adjacent to urban and agricultural settings. One key measurement was water column respiration, assayed using *in situ* dark bottle incubations. We found that water column respiration increased with stream order. This is counter to previous work showing that CO_2 (a product of respiration) evasion from streams decreases with increasing stream order. This also implies that the fraction of ecosystem respiration from sediments may decrease with stream order. If so, that would reject current model predictions; a field campaign in summer 2022 will test this hypothesis and outcomes will guide model refinements and updated model predictions. Further, our work both rejects and supports the River Continuum Concept (RCC). The RCC predicts that organic matter (OM) chemistry will vary down the stream network. Consistent with the RCC, OM diversity increased down the network. In contrast, processes governing OM chemistry were similar at the top and bottom of the network, but distinct in the middle. These results point to a need to revise some of the conceptual and mechanistic foundations of river corridor hydrobiogeochemistry.

Improving Knowledge and Predictions of Hyporheic Zone Respiration via Continental-Scale Iterative ICON-ModEx Science

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Project Abstract: *This element of the PNNL River Corridor SFA is focused on improving predictive understanding of hyporheic respiration.* The Earth's biogeochemical and water cycles are tied closely to river corridors and stream respiration. Microbes in hyporheic sediments have a wide range of influence over river corridor biogeochemistry; hyporheic zones contribute from 4 to 96% of stream respiration. This project addresses the uncertainty of predicting this variation. We are combining public data, artificial intelligence (AI) and mechanistic modeling, ICON principles, and model-experiment (ModEx) iteration via crowdsourced sampling across the contiguous United States (ConUS). ICON principles, facilitated via the ICON Science Cooperative, are used by Integrating AI modeling with biogeochemistry, Coordinating protocols to be consistent with previous efforts, Openly sharing ideas and data, and Networking with stakeholders to increase mutual benefit of outcomes. The project started with data from the Worldwide Hydrobiogeochemical Observation Network for Dynamic Rivers (WHONDRS) to develop a suite of AI models to predict respiration rates at unsampled locations across the ConUS. Due to limited data, the model has biased predictions at high respiration rates. The project is working to improve the model and determine which variables drive hyporheic zone respiration rates. To address inaccuracies in model predictions, we guide volunteers to high priority locations across the ConUS for new sample collection. Both open stakeholder engagement and model needs will determine sample collection and data generation. Results will be fed back into the model to make new predictions and guide additional sampling, with the aim of multiple ModEx iterations. Once the respiration model is refined, it will be incorporated into basin-scale mechanistic hydro-biogeochemistry modeling, which will quantify how basin-scale fluxes of carbon and nutrients are impacted by variation in hyporheic respiration.