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Pacific Northwest National Laboratory SFA Annual Report

River Corridor Hydrobiogeochemistry from Reaction to Basin Scale

June 2023

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PNNL River Corridor Scientific Focus Area Annual Report FY2023

River Corridor Hydrobiogeochemistry from Reaction to Basin Scale

2023 Annual Report

June 30, 2023

TABLE OF CONTENTS

I. PROGRAM OVERVIEW

The Pacific Northwest National Laboratory (PNNL) River Corridor Science Focus Area (SFA) is transforming understanding of spatial and temporal dynamics in river corridor hydrobiogeochemistry from reaction to watershed and basin scales, enabling mechanistic representation of river corridor processes and their responses to disturbances in multiscale models of integrated hydrobiogeochemical function.

Our research is focused on understanding the controls on spatial and temporal variations in river corridor hydrobiogeochemistry, hydrobiogeochemical responses to wildfires and other disturbances, and representation of river corridor hydrobiogeochemistry in numerical models from reaction to basin scales. The project's goals are aligned with the objective of DOE's Office of Biological and Environmental Research (BER) to improve scientific understanding and prediction of the function of natural and managed watersheds and their responses to disturbances.

Our long-term vision is to mechanistically link the impacts of disturbance on hydrologic exchange flows (HEFs, the exchange of water between surface and subsurface environments in river corridors), molecular processes, and biogeochemistry to watershed function across CONUS basins. This vision is being achieved through distributed, basin-scale science pursued via extensive collaboration with the research community following ICON-FAIR principles (DOE, 2019). These principles focus on doing science by-design that **I**ntegrates physical, chemical, and biological processes, is **C**oordinated via consistent methods from field to lab to analysis, uses **O**pen science methods such as making data FAIR, and is **N**etworked with the community to enable distributed data generation and modeling that are mutually beneficial to all. Our hypothesis-driven approach advances transferable understanding of coupled hydrobiogeochemical processes through integrated multiscale experiments, observations, and modeling. Enabling mechanistic representation of river corridor processes from reaction to watershed and basin scales will provide a foundation for developing the next generation of watershed models with enhanced predictive capacity to inform watershed management strategies aimed at solving the nation's environmental challenges in the face of extreme disturbances.

Progress toward this vision is achieved through four Research Campaigns (RCs) integrated through a Multiscale ModEx approach as shown in Figure 1, in keeping with the concept of iterative model-driven experimentation and observation. SFA team members work on multiple campaigns, campaign activities are jointly coordinated by the PI team, and high-impact publications are targeted that integrate information across the four campaigns to address high-level project objectives.

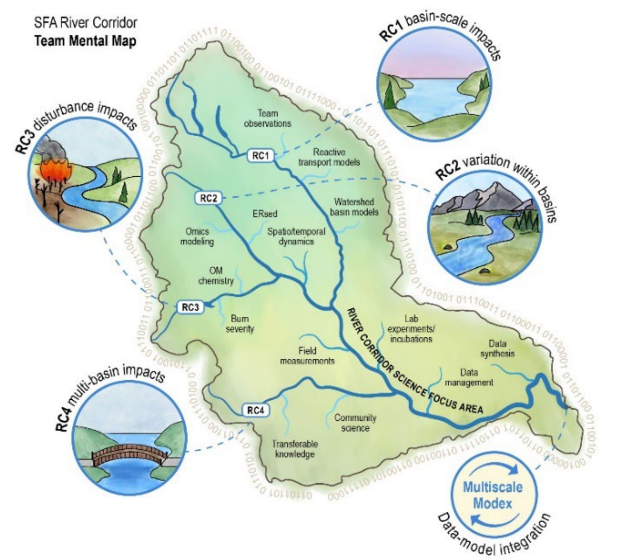

Figure 1. The "Team Mental Map" of the River Corridor SFA, in which Research Campaigns (RCs) are represented as major rivers in the Yakima River Basin (YRB), and characteristic activities are denoted as sub-catchments. Multiscale Modex is an iterative data-model learning loop in which models and experiments across scales are co-designed to test central hypotheses and develop predictive understanding.

- The *Cumulative Effects Campaign* (RC-1) aims to reveal the cumulative effects of river corridor processes and their appropriate representations in watershed- and basin-scale models.
- The *HBGC Variability Campaign* (RC-2) aims to elucidate interactions among hydrologic and molecular processes that control the cycling of nutrients (N, P), dissolved organic

matter (DOM), and inorganic contaminants (e.g., NO_3^-) in river corridors from reaction to basin scales.
- The *Watershed Disturbances Campaign* (RC-3) aims to reveal the mechanisms by which wildfires impact biogeochemical cycling in river corridors from reaction to basin scale.
- The *Multi-Basin Studies Campaign* (RC-4) aims to provide transferable principles that integrate DOM chemistry, microbial gene expression, biogeochemical function, and disturbance by combining existing global-scale data with Worldwide Hydrobiogeochemistry Observation Network for Dynamic River Systems (WHONDRS)-based data generation and numerical modeling distributed across CONUS basins.

II. KEY SCIENTIFIC OBJECTIVES

In keeping with the vision outlined above, we have expanded both the physical scale and complexity of our research while maintaining our focus on the study of HEFs, DOM chemistry, microbial activity, and associated biogeochemical processes in the river corridor and their cumulative impacts at watershed and basin scales. The physical scope of our study focuses on the Yakima River Basin (YRB, Figure 1), a major sub-basin of the Columbia River Basin encompassing an area of 15,900 km^2 in which there exists a wide range of stream orders (1 to 8) and a variety of physiographic watershed settings. This large-scale study domain has provided new opportunities to study broadly distributed disturbances and their impacts across diverse environmental conditions. Our work focuses on impacts of wildfire and hydrologic intermittency on river and watershed hydrobiogeochemistry, while spanning gradients in climate, vegetation, land use, and other key watershed features to increase the transferability of our scientific findings. We aim to further extend the transferability of our science by studying multiple basins across the CONUS using ICON-based community science methods. Our research is structured around the scientific grand challenge defined below.

Scientific Grand Challenge: Understand and quantify processes governing the cumulative effects of HEFs, DOM chemistry, microbial activity, and disturbances on river corridor hydrobiogeochemical functions at watershed to basin scales.

Dynamic HEFs are a primary driver of river corridor biogeochemistry, which is highly sensitive to DOM chemistry and microbial activity (e.g., expressed metabolic pathways). Disturbances such as wildfire and stream intermittency interact to create feedbacks among physical and biogeochemical processes. These concepts motivate both fundamental process studies and the development/implementation of a multiscale modeling framework, and lead to the following SFA-level science questions that guide our research plan:

Overarching Science Questions:

1. How do HEFs, DOM chemistry, microbial activity, and disturbances interactively influence river corridor hydrobiogeochemical function from reaction to basin scales?
2. How can mechanisms that govern river corridor hydrobiogeochemistry be efficiently and sufficiently represented in integrated land surface models at scales relevant to regional and national water challenges?

III. PROGRAM STRUCTURE

The PNNL SBR-SFA is led by a Principal Investigator (PI, Tim Scheibe) and two Co-PIs (Xingyuan Chen and James Stegen) (Figure 2). In his role as Director of Program Development for PNNL's Earth and Biological Sciences Directorate, Scheibe also serves as the primary point-of-contact with the DOE-BER. The SFA is organized around four RCs (Figure 1), each of which is led or co-led by one of the three PIs. An early career staff member, Allison Myers-Pigg, is co-leading RC-3 with mentorship from PI Scheibe, with the expectation of her development into a co-PI position over time. Each RC comprises two to three major activities; each activity is organized into several Sub-Activities. The

Multiscale ModEx (MM) cross-cutting activity serves an integrating role to ensure that observational, experimental, and modeling research are highly coordinated. Activity Leads are responsible for coordinating research within each activity and are members of the SFA Leadership Team. Other key staff have responsibilities within one or more activities or sub-activities and contributing staff (including funded collaborators) are disciplinary experts that lead or contribute to one or more activities. SFA researchers are drawn from multiple research directorates at PNNL as dictated by the interdisciplinary nature of SFA research. The RCs, activities, and sub-activities have been jointly designed and are closely coordinated by the Leadership Team to accomplish overall project scientific objectives.

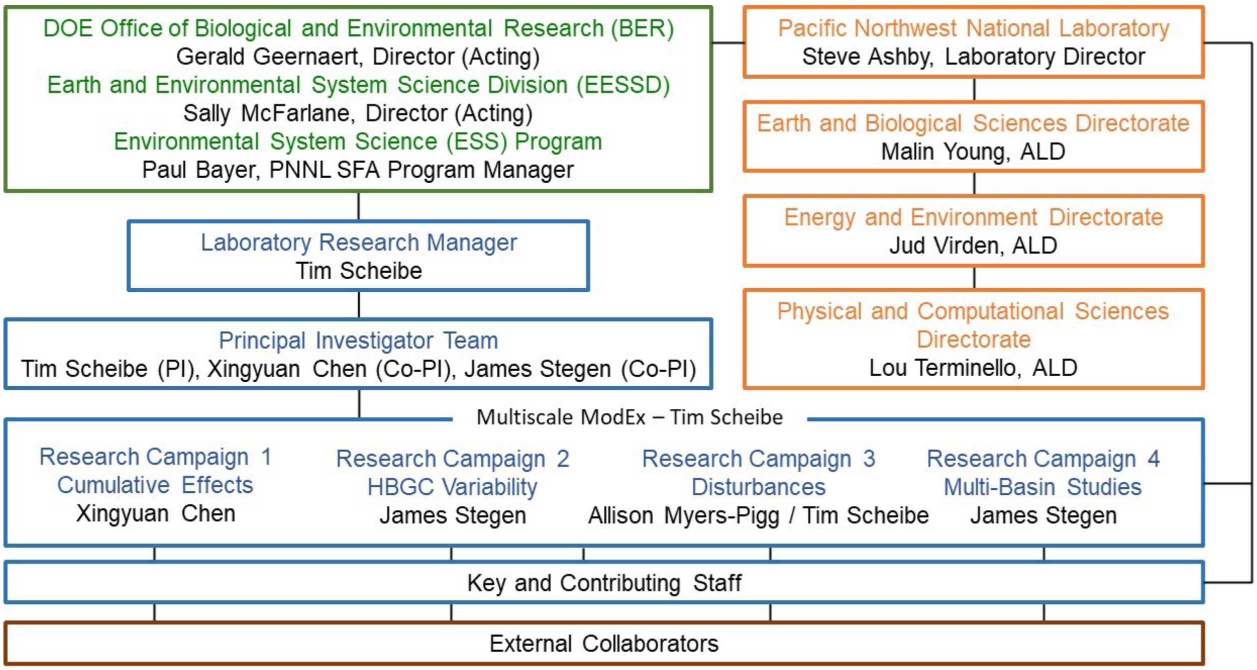

Figure 2. PNNL River Corridor SFA organizational structure.

Our management philosophy and process are characterized by 1) intentional, regular and transparent communication and documentation of progress and 2) emphasis on individual awareness of and accountability to team outcomes. This, in the context of our team values of scientific excellence, creativity, collaboration, and mentorship, leads to active engagement of the entire project team in pursuing the integrated objectives of the project. Primary avenues for team coordination and communication are: 1) regular meetings at a variety of organizational levels, and 2) extensive utilization of collaborative environments including Microsoft Teams (virtual meetings, file sharing, persistent chat), Atlassian Confluence (wiki), AirTable (task tracking), GatherTown (virtual workspace), and others. We are actively learning and applying principles of the Science of Team Science (SciTS) (NRC, 2015) to enhance transdisciplinary integration and teaming within the project and with external collaborators. For example, Figure 1 is a representation of the SFA "Team Mental Map" - a graphical representation of the mental model of the research objectives and collaborative structure shared by team members (Cannon-Bowers et al., 1993). Research in the SciTS field has shown that shared mental models enhance the effectiveness of science teams and other larger groups. Figure 1 was developed based on input from all team members and discussion of individuals' mental models of the project and is used in many contexts to communicate the overall project objectives and approach.

IV. PERFORMANCE MILESTONES AND METRICS

Review of Scientific Progress Toward Program Objectives and Milestones

Research Campaign 1 (RC-1): Cumulative Effects

Overall Objectives: *The Cumulative Effects Campaign aims to reveal the cumulative effects of river corridor processes and their appropriate representations in watershed- and basin-scale models.*

- Quantify baseline cumulative effects: Quantify the cumulative effects of river corridor HEFs, DOM chemistry, and microbial activity on watershed and basin biogeochemical cycling, water quality (including temperature), contaminant mobility, and land surface fluxes. Use reaction network models and rate kinetics developed from lab and field studies in RC-2 to inform river corridor reactive transport models.
- Quantify cumulative effects of disturbances: Reveal the cumulative impacts of wildfire and precipitation on watershed- to basin-scale hydrobiogeochemical functions of river corridors. Leverage new reaction networks and kinetics, focusing on the effects of wildfire-affected DOM chemistry on river corridor metabolism developed in RC-3 in coordination with RC-2.
- Guide field and lab experiments: Provide basin-scale river corridor model outputs of biogeochemical hot spots and hot moments to focus field and laboratory experiments of RC-2 and RC-3 in locations and time windows that are most effective at reducing uncertainties in watershed model predictions.

Key Contributions of this Research Campaign to the SFA: RC-1 is integrating numerical models developed at multiple scales with distributed monitoring in other RCs across the YRB to advance predictive understanding of emergent system behaviors arising from complex hydrobiogeochemical interactions. We are building a watershed- to basin-scale river corridor model that links dynamic flow processes with variable temperatures and reaction kinetics (informed by molecular properties) to investigate water, energy, and mass fluxes across the river-groundwater interface. This model will be used to further quantify the cumulative impacts of HEFs, molecular properties, and disturbances on the watershed- and basin-scale biogeochemical cycling of key nutrients (C, N, P) and inorganic contaminants (e.g., NO_3^-).

FY23 Science Plan Milestone: Incorporate new molecular and biogeochemical understanding from RC-3 with wildfire-impacted watershed hydrology to evaluate the impacts of wildfire on river corridor biogeochemistry. Evaluate impacts of DOM molecular properties and microbes on river corridor biogeochemistry post wildfires in the YRB. Evaluate impacts of burn severity and precipitation scenarios on watershed hydrology and stream biogeochemistry in the YRB.

Progress Brief for FY23: Our activities in FY23 are focused on (1) developing ATS-PFLOTRAN coupled hydrobiogeochemical models for selected watersheds within YRB; (2) evaluating impacts of burn severity and precipitation scenarios on watershed hydrology and stream biogeochemistry in the YRB; (3) examining the variations in reaction mechanisms across YRB using distributed molecular characterization performed by RC-2 and incorporate this variability into watershed HBGC models; and (4) understanding how ecosystems recover from fires using remote sensing data products. We have made significant progress in fixing various numerical issues in adopting ATS-PFLOTRAN for watershed hydrobiogeochemical simulations. We are poised to examine watershed biogeochemical responses under a range of environmental conditions and disturbance scenarios.

Evaluating watershed hydrologic responses to wildfires in the Pacific Northwest using high-resolution numerical models. The escalating frequency and severity of wildfires in the Pacific Northwest region have been widely acknowledged. Wildfires exert substantial influence on the physical properties of soil, leading to the occurrence of Soil Water Repellency (SWR) due to the formation of a hydrophobic layer post the burning. We developed a novel fire module within the ATS-PFLOTRAN modeling framework to account for fire-induced SWR. The models were set up at high temporal resolution (hours) and spatial resolution (tens of meters) to fully capture the dynamics in watershed responses. The model inputs encompassed extensive hydrographic, geologic, ecological, and climatological data from publicly accessible sources such as the National Land Cover Database (NLCD), Soil Survey Geographic Database (SSURGO), Daymet, among others. The Monitoring Trends in Burn Severity (MTBS) data were used to quantify the reduction in top-layer soil permeability post fires. We studied the American River Watershed (Norse Peak Fire in 2017), Wenas Creek Watershed (Evans Canyon Fire in 2020), Naches River Watershed (Schneider Springs Fire in 2021), and Mckenzie River Watershed (Holiday Farm Fire in 2020) across a range of burn areas and severities. Our modeling results reveal that medium to severe wildfires could increase the peak surface runoff after accounting for the SWR effects. The increase in peak flow was found to increase nonlinearly with the post-fire precipitation intensity. Furthermore, we found that fires with low average burn severity only led to negligible differences in peak discharge induced by SWR. Fire-induced reduction in Manning's surface roughness was found to have much more significant impact on the post-fire peak discharges at the watershed outlets.

Integrating carbon speciation data generated from FTICR-MS into reactive transport models. In collaboration with the IDEAS-Watersheds project, we integrated substrate-explicit modeling (Song et al., 2020) (deemed the lambda model) which characterizes individual organic matter reactivity based on thermodynamics with PFLOTRAN's reaction sandbox to enable the understanding of spatial variability in DOM characteristics across the YRB using the RC2 spatial studies. We first implemented the governing expressions of the lambda model, which also built in flexibility to handle variations in FTICR-MS data and analysis configurations. Upon implementing within PFLOTRAN, we developed a pipeline within a Jupyter Notebook that digests raw FTICR-MS data, calculates the lambda distribution for the sample, generates the corresponding reaction network, and completes a biogeochemical simulation using PFLOTRAN. We have also developed sensitivity analysis and parameter estimation capabilities, allowing a user to confront batch simulation results with incubation experimental data for hypothesis-driven ModEx iterations. The governing reaction rate expressions were updated to include reactant inhibition and microbial biomass carrying capacity. We were able to batch process the FTICR-MS datasets provided by the RC2 team to understand the variability in carbon species across YRB and understand the variability in batch responses regarding the aerobic respiration. Such reactivity variability will be incorporated into watershed-scale hydrobiogeochemical simulations by developing new capabilities in ATS-PFLOTRAN that allows spatially variable rate parameters.

Understanding topographic and climatic controls on post-fire vegetation recovery across different burn severity and land cover types in the Pacific Northwest. While forests recover over time after wildfire occurrences, the recovery pattern depends on complex interactions between several topographic and climatic conditions. Despite efforts to understand such interactions, the varying impact on different land cover types associated with varying burn severity remains unexplored. We investigated the interplay between topography, post-fire climate conditions, burn severity and years after fire on vegetation recovery across the dominant land cover types (evergreen forest, shrubs and grassland) in the Pacific Northwest (PNW) region. All PNW burn areas in 2015, except grids experiencing fire occurrences after 2015, were analyzed. To estimate vegetation recovery during post-fire years (2016-2022), incremental enhanced vegetation index (EVI) was calculated using EVI data from Moderate Resolution Imaging Spectroradiometer (MODIS), which are available at 250 m spatial resolution every 16 days. Climate, topographic, burn severity and land cover data were collected from Daymet, USGS, MTBS and NLCD, respectively. Machine learning methods, including the random forest (RF) and XGBoost, were employed to map relationships between the input features (elevation, slope, aspect, precipitation, temperature, burn severity and years after fire) and target, incremental EVI recovery. The models were trained using 75% of the MODIS grid cells within the Columbia River Basin and tested using the other 25% of grid cells. Partial dependence plots (PDP) were generated to understand the influence of each feature and combination of feature pairs on predicted incremental EVI. Preliminary results showed that both RF and XGBoost significantly outperformed the multiple linear regression, indicating the importance in capturing the nonlinear relationships between the input features and ecosystem recovery. Nash–Sutcliffe efficiency (NSE) and Kling-Gupta efficiency (KGE) values for total recovery predicted by the XGBoost models were above 0.9 and 0.84 for the training and testing sets, respectively. Permutation and drop one variable feature importance revealed year after fire and precipitation were the most important features. Among the topographic features, elevation was the most important, impacting EVI recoveries for all three land cover types. For evergreen forest, higher recovery was found in the east and south aspects. However, impact of aspect was insignificant on EVI recovery for shrubs and grasslands. Among all the input features, slope was found to have the least impact on EVI recovery across all three land cover types. This exploratory study has generated new understanding of the mechanisms that may control the ecosystem recovery from different fires, shedding new light on modeling such recovery using process-based models such as ELM, the land surface model of the E3SM family.

Publication Highlight: A newly developed basin-scale river corridor model can quantify the spatial variation of hyporheic zone respiration of the reaches in the Columbia River Basin (CRB).

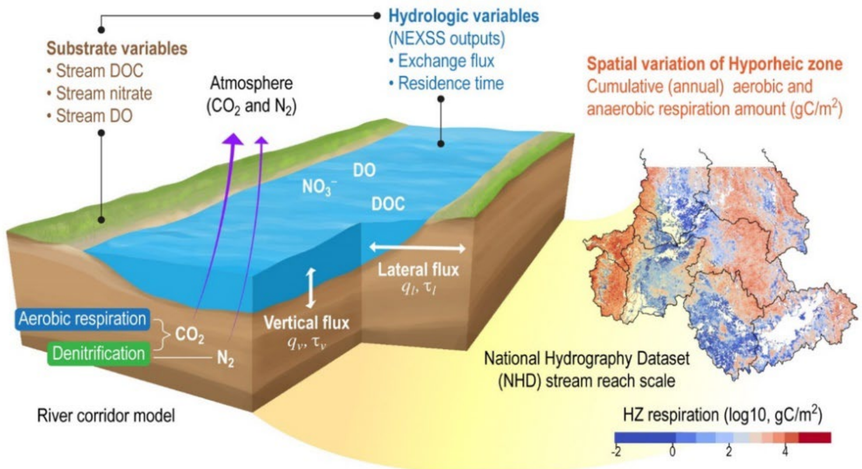

Figure 3 The river corridor model (RCM) and its key processes.

While the hyporheic zone (HZ) accounts for a significant portion of whole stream CO_2 concentrations, HZ respiration modeling studies are lacking in quantifying their contributions to the total CO_2 at large watershed/basin scales. Quantifying the contribution of anaerobic respiration is also underappreciated. This study developed a basin-scale coupled carbon-nitrogen river corridor model to quantify HZ aerobic and anaerobic respiration and determined the key factors controlling their spatial variability within the Columbia River Basin (CRB). A numerical simulation model (Figure 3) was used to estimate CO_2 emissions from riverbeds into water columns in the presence and absence of oxygen and identified important variables explaining the spatial variation of riverbed CO_2 emissions within the CRB. Our modeling study found that CO_2 emissions from riverbeds showed high spatial variability. Within the CRB, wetter sub-basins showed higher CO_2 emissions than drier sub-basins. Medium-sized rivers generated the highest CO_2 emissions. Most channel CO_2 emissions occur in the presence of oxygen. However, reaches in agricultural lands generated relatively high CO_2 emissions without oxygen. The water exchange rate between channel and riverbed can explain the spatial variation of CO_2 emissions over other physical variables.

Reference: Son, K., Fang, Y., Gomez-Velez, J.D. and Chen, X., 2022. Spatial microbial respiration variations in the hyporheic zones within the Columbia River Basin. *Journal of Geophysical Research: Biogeosciences*, *127*(11), p.e2021JG006654.

Plans for FY24: In FY24, we will focus on (1) developing ATS-PFLOTRAN models for YRB with spatially variable reaction mechanisms informed by FTICR-MS characterization; (2) deriving reaction networks in fire-impacted watersheds (collaborating with RC-3) and incorporating them into ATS-PFLOTRAN models to investigate the impacts of fire on the HBGC regimes in river corridors; and (3) using watershed-scale hydrobiogeochemical models to generate new hypothesis for RC2 and RC3 field-based studies.

Research Campaign 2 (RC-2): Hydrobiogeochemical Variability

Overall Objectives: The HBGC Variability Campaign aims to elucidate interactions among hydrologic and molecular processes that control the cycling of nutrients (N, P), DOM, and inorganic contaminants (e.g., NO 3−) in river corridors from reaction to basin scales.

- Identify important places/times: Use NEXSS and SPARROW predictions (existing and from RC-1.1) to guide placement of in situ sensors to span a range of predicted respiration contributions of sediment-associated microbes (ERsed), relative to those in surface water. Use to identify where and when ERsed is disproportionately high.
- Compare to predictions: Compare field-estimated ERsed to NEXSS predictions and use outcomes to inform structure of and parameterize basin-scale models in RC-1.1.
- Characterize variation: Use field surveys across reaches that differ in ERsed to characterize longitudinal and seasonal variation in DOM chemistry, microbial gene expression, and nutrient concentrations in surface and pore water.
- Inform models: Use field survey data to inform 1-D reactive transport models that predict biogeochemical rates using explicit representation of DOM chemistry, microbial gene expression, and nutrient concentrations.
- Understand consequences: Use RC-1 models and field surveys to guide lab experiments to reveal influences of DOM chemistry, microbial gene expression, and nutrient concentrations on biogeochemical rates predicted by reactive transport models.
- Refine models: Use experimental outcomes to test and refine substrate/microbe-explicit reaction network models, use these models to evaluate impacts of PyOM in collaboration with RC-3, and integrate them into reactive transport models in collaboration with RC-1.

Key Contributions of this Research Campaign to the SFA: The SFA is designed to increase predictive understanding of the variations in river corridor hydrobiogeochemical processes across stream orders as well as other climatic, ecological, and geographic settings. RC-2 has started to elucidate interactions among hydrologic and molecular processes that control the cycling of nutrients (N, P), DOM, and inorganic contaminants (e.g., NO_3^-) in river corridors by initiating a series of ModEx-based sampling and monitoring campaigns across the YRB. As these campaigns generate data sets spanning both long periods of time and a broad variety of geographic settings, they provide the basis for both exploring the mechanistic linkages between process and setting, as well as iteration with numerical models to improve predictive ability.

FY23 Science Plan Milestone: The FY23 milestone has been revised to focus more on basin-scale ModEx needs within the YRB, which we feel are vital to address in order to first understand large-scale patterns, prior to diving into finer-scale mechanisms. Evaluate model-generated hypotheses via analysis of time series data from sensors and samples from across multiple biomes within the YRB, and complement with spatially distributed analyses of temporally static properties that are critical inputs to RC-1 models. Coordinate with RC-3 and RC-4 on field site locations to maximize co-use of sites/data across multiple research campaigns.

Progress Brief for FY23: Our activities in FY23 are focused on multiple basin-scale ModEx efforts that span river corridor biogeochemical rates, physical properties, and DOM chemistry, along with enhanced stakeholder engagement and development of new measurement capabilities.

Field measurements in the Yakima River Basin address basin-scale science questions and support model parameterization. We continued our ~3-year program of temporal sampling (focused on stream chemistry) of 6 stream locations across the YRB, a mature/routine monitoring effort generating data that are needed by RC-1 models and useful for evaluating basin-scale science questions. For example, we found a striking basin-wide scaling pattern in which DOM transformations in surface water increase with catchment area, which suggests that larger areas with diverse landcover result in diverse organic matter functions (Danczak et al. 2023). We initiated an effort to increase the coverage and accuracy of median particle size distributions (d50) estimates across the YRB using field photos. Sediment d50 is the key physical variable governing CO_2 production and fluxes across the YRB stream network. Initially, we selected 11 photos, generated 4,315 labels, and trained a You Look Only Once (YOLO) AI model with R^2 = 0.89. We compared these estimates to CONUS-scale model estimates and direct measurements of d50, and found major differences (Regier et al., in prep). We then improved the YOLO accuracy using 61 additional photos, achieving R^2 = 0.97. The improved model was used to quantify d50 for 2148 more photos from across the YRB, and we further used those photos to estimate hydrologic (e.g., exchange fluxes) and biogeochemical (e.g., nitrate uptake) parameters at all photo locations (Chen, Y. et al., in prep.). We also quantified particulate organic matter (OM) decay rates across the YRB (in the same locations used for sediment respiration measurements) using cotton strip decomposition as a standardized assay that integrates environmental and microbial processes. Measured decomposition rates showed high variation in across the basin and spanned globally observed rates. Decomposition was fastest in higher stream orders where carbon and nitrogen concentrations were elevated, temperatures were greater, and land use was dominated by agriculture. Decomposition was fastest in locations with greater fine-grain sediment respiration, but with lower whole-river respiration. The broad range of observed decomposition rates support the YRB as a model study system to gain mechanistic understanding of river corridor metabolism and indicate that decomposition is influenced by some, but not all, of the same features that impact sediment respiration. The SFA has made important advances in field and laboratory measurement methods. We developed the "metabolic multireactor" (Kaufman et al. 2023), which allows for multiple small bioreactors to be operated simultaneously and their DO concentrations to be measured at high time resolution providing high-throughput allowing greater spatial sample coverage. We also published a methods paper on the use of inexpensive open-source sensors, showing that they provide data of equal or better quality than commercial sensors (Fulton et al. 2023).

Analysis and modeling of YRB measurements reveals basin-scale patterns of hydrobiogeochemical function. We analyzed data from 2021, spanning ~60 YRB locations, to demonstrate that water column respiration is a minor contributor to river corridor ecosystem respiration across all YRB biomes (Fulton et al., in prep). While variability in water column respiration could be largely (>70%) explained by total N, temperature, and drainage area, median rates were 680 times slower than whole river ecosystem respiration rates (which include sediment contributions) compiled from literature, underscoring the importance of understanding and modeling mechanisms and patterns of sediment-associated respiration. Spatial patterns in sediment respiration rates were identified through analyses of field measurements of dissolved oxygen and other metabolism-related parameters at 48 sites across the YRB and used to test model-generated hypotheses regarding spatial patterns. We ran DO timeseries through a Bayesian inversion to estimate ecosystem respiration and paired those data with *in situ* measurements of water column respiration to estimate (by difference) the sediment-associated respiration. This analysis revealed that >98% of ecosystem respiration was sediment-associated, consistent with the results of Fulton et al. (in prep), and identified YRB respiration hot spots, which were largely explained by stream slope and velocity -- hot spots occurred in streams that are low gradient, slow flowing, and ag-impacted. We applied meta-metabolome ecology to reveal that mid-order streams are domains of enhanced DOM processing. We observed non-random forces driving DOM chemistry along the river continuum. Specifically, we observed that mid-sized streams experienced the most non-random processes influencing DOM chemistry. These results support the recently proposed Bending DOM Concept which suggests that both spatially structured variables and biological activity have their strongest influences of DOM chemistry in mid-sized streams. We found mixed support for theoretical expectations for the relationship between upstream drainage area and cumulative sediment respiration rates. These analyses were done using RC-1 model outputs across the YRB and the Willamette Basin (similarly sized but hydrologically contrasting basins). Analyses indicate that strong scaling is found only within specific land-use categories and within small ranges of hyporheic zone residence times. We infer that current scaling theory is incomplete and requires elaboration via consideration of spatially variable inputs and riverbed physical properties (Guerrero et al., in prep.).

Community Engagement and Support. We developed and deepened relationships with a variety of stakeholders. Within the YRB we have held multiple discussion with Yakama Nation fisheries aimed at understanding their needs and identifying strategies for mutual benefit (e.g., selecting field sites that have value to both RCSFA and Yakama Nation). Our temporal sampling locations (described above) are paired with stream gauges operated by other agencies to provide mutual benefit. We have pursued new collaborations within and beyond the YRB through public engagements, proposal partnerships, and training (see Appendix B for details). We published multiple FAIR data packages[1] on ESS-DIVE using ESS-DIVE Reporting Formats, often prior to data use/analysis. These data packages are primarily YRB-focused, contain more than 25 different data types, and require optimizing strategies to meet the needs for rapid data access and for high-quality FAIR data.

Publication Highlight: Metabolism patterns in the Columbia River contrast with smaller rivers.

Rivers are a major component of the Earth system. The study of river metabolism is key for understanding nutrient dynamics, overall system health and biodiversity and habitat quality in river ecosystems. This study focuses on understanding ecosystem metabolism in large rivers, an area that has received limited attention compared to small and medium rivers. Large rivers present unique challenges for measurements due to their size, including depth measurements, gas exchange estimations, and the presence of large dams that affect gas levels. Here, we estimate reach-scale metabolism for the Hanford Reach of the Columbia River in Washington state, a free-flowing stretch with a substantial discharge (Figure 4). We overcome some of the limitations of gas exchange estimates driven by large dams by calculating exchange rates from semi-empirical models and tracer tests. Overall, the results showed that metabolism metrics were comparatively high in the Columbia River, with peak values occurring in late summer or early fall. The river exhibited plankton-dominated metabolism driven by light availability and temperature. The study highlights that metabolism patterns in large rivers, such as the Columbia River, differ from those observed in small-medium rivers, and requires the application of knowledge and tools beyond those implemented for smaller rivers.

Reference: Roley, S., R. Hall, W. Perkins, V. Garayburu-Caruso, J. Stegen. 2023. "Metabolism patterns in the Columbia River contrast with smaller rivers," accepted for publication in *Limnology and Oceanography.*

Plans for FY24: (1) Continue to publish data packages on ESS-DIVE using reporting formats as early as possible in the research life cycle. (2) Complete evaluation of RC-1 model-generated hypotheses for spatial variation of sediment respiration and develop a new conceptual model/hypothesis based on deviations from the model-generated hypotheses. (3) Complete numerous publications, summarized above, based on field and lab efforts across the YRB. (4) Conduct targeted field campaigns focused on mechanistically understanding what leads to YRB-scale hot spots of sediment respiration, with an emphasis on evaluating the role of algal biofilms and submerged vegetation, and provide outcomes to RC-1 to inspire inclusion of additional physics in mechanistic models.

[1] https://data.ess-dive.lbl.gov/view/doi:10.15485/1971251; https://data.ess-dive.lbl.gov/view/doi:10.15485/1898914; https://data.ess-dive.lbl.gov/view/doi:10.15485/1969566; https://data.ess-dive.lbl.gov/view/doi:10.15485/1898912; https://data.ess-dive.lbl.gov/view/doi:10.15485/1892054; https://data.ess-dive.lbl.gov/view/doi:10.15485/1892052; https://data.ess-dive.lbl.gov/view/doi:10.15485/1923689; https://data.ess-dive.lbl.gov/view/doi:10.15485/1972232; https://data.ess-dive.lbl.gov/view/doi:10.15485/1971118

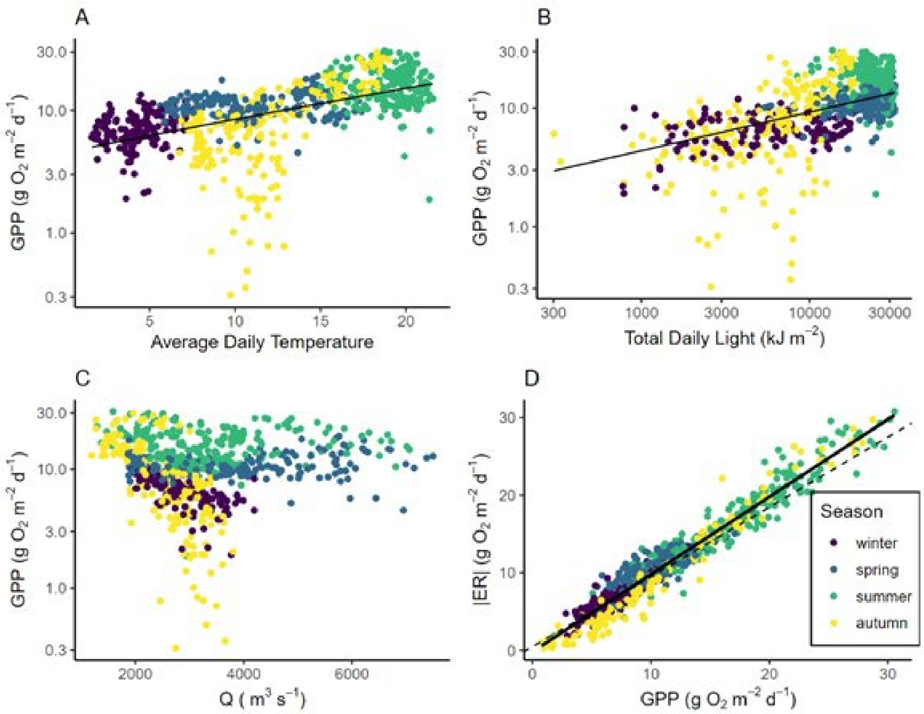

Figure 4 Drivers of metabolism in the Hanford Reach: A) average daily temperature expressed in C; B) total daily light expressed in kJ/m2; C) discharge (Q); and D) the relationship between ER and GPP. Note that (A) and (B) are plotted on a log scale. The fitted lines were fit via gls with a corAR1 autocorrelation structure, except (D) which was fit with a linear model. The dashed line in (D) shows the fraction of GPP that is immediately respired, fit with quantile regression at the 0.9 quantile.

Research Campaign 3 (RC-3): Watershed Disturbances

Overall Objectives: *The Watershed Disturbances Campaign aims to reveal the mechanisms by which wildfires impact biogeochemical cycling in river corridors from reaction to basin scale.*

- Identify impacts of burn severity: Identify the impacts of burn severity on relationships between pyrogenic material (e.g., PyOM and inorganic nutrients) and river corridor biogeochemistry, with an emphasis on lab-based activities based on BER guidance for changes in RC-3 scope.
- Derive PyOM indicators: Reveal biogeochemical indicators of PyOM derived from different burn severities that can be used for multiscale characterization of PyOM distributions.
- Understand temporal trajectories: Advance the understanding of temporal trajectories of biogeochemical impacts of wildfires within river corridors and their relationship to precipitation.
- Develop PyOM reaction networks: Incorporate the processing of pyrogenic material into reaction network models.
- Relate pyrogenic impacts to watershed features: Lay a foundation for understanding dynamic relationships between pyrogenic materials and river corridor biogeochemistry across variation in watershed features (e.g., stream order and discharge, upland soil physical properties, evapotranspiration, slope of surrounding landscape, and burn area).

Key Contributions of this Research Campaign to the SFA: The River Corridor SFA integrates understanding on the controls of spatial and temporal variations in river corridor hydrobiogeochemistry, its responses to disturbances, and representation in numerical models from reaction to basin scales. To robustly predict changes in watershed function in response to wildfire disturbances, and how those changes will affect water quality and ecosystem health, RC-3 is working on developing a mechanistic understanding of governing processes on the impacts of fires on river corridor hydrobiogeochemistry and is working with RC-1 to further improve model predictive capacity in watersheds impacted by fire disturbances, important for ascertaining the impact of fire on ecosystem structure and function.

FY23 Science Plan Milestone: *In accordance with the changes in budget and scope based on BER guidance, the updated FY23 milestone is as follows:* Continue to establish the chemical composition of burned substrates and define associated PyOM indicators in the context of burn severity, focusing on characterizations of PyC, PyP, and PyN. Collect spatially distributed samples to understand the influence of wildfires on river respiration rates, in collaboration with RC-2. Collaborate with RC-1 to incorporate wildfire dynamics into predictive models.

Progress Brief for FY23: Our activities in FY23 are focused on furthering understanding of burn severity on wildfire influences across ecosystem types and increasing understanding of field scale in-stream responses to fires.

Chemical composition of burned substrates and associated PyOM indicators in the context of burn severity. In FY23, we have deepened our understanding of carbon (C), nitrogen (N), and phosphorus (P) chemical species change with changing burn severities across different ecosystem types (represented experimentally by vegetation types). Solid char quality suggests no major shift in C/N ratios but greater C & N limitation relative to P with increasing burn severity. We have established that vegetation/ecosystem type is a co-determinator of the impact different burn severities have on C, N, and P chemistry; for example, the leachability of C, N and P varies with burn severity and ecosystem type. Increasing burn severity created systematic shifts in P biogeochemistry where a loss of organic species and higher proportion of inorganic calcium-bound species (identified by nuclear magnetic resonance, NMR and X-ray absorption near edge structure, XANES) resulted in less export of P in the soluble phase and greater mobilization of particulate bound P. These results indicate a transformation to the potential export and reactivity of P in the environment post wildfire (Barnes et al., in prep). As a part of this activity, we have published multiple versions of a FAIR data package[1] on ESS-DIVE using ESS-DIVE Reporting Formats, prior to data use/analysis. Versioning of the data package allows for greater accessibility and transferability of these research outcomes, by maintaining a single DOI across the entire experiment's outcomes. The two versions of this data package that have been published in FY23 contains more than 10 different data types, including some produced via our EMSL Large Scale User proposal (NMR and FTICR-MS datasets).

In FY23, team members traveled to the Canadian Light Source (CLS) as a part of a user proposal awarded in FY22. At CLS, we collected XANES datasets for C and N chemistry to complement XANES results collected from the Stanford Synchrotron Radiation Lightsource (SSRL) for P chemistry. These results are being processed and prepared for publication (Roebuck et al., in prep; Torgeson et al., in prep). A DOE SCGSR was awarded to Riley Barton to work with the RC-3 team to establish a high-throughput method for the pyrogenic molecular marker, levoglucosan, a complementary method to the PyOM molecular composition work currently conducted by the RC-3 team. Riley will begin work at PNNL in October 2023. We also completed a comparative analysis on sample preparation for FTICR-MS analysis in collaboration with RC-2, to assess methodological biases that may exist and to compare these results to optical properties on whole water samples (Roebuck et al., in review; see highlight below). This work is relevant for the potential development of in-stream optical sensors that could allow greater extrapolation of high-resolution molecular information from river networks across spatial and temporal scales.

Understand the influence of wildfires on the spatial and temporal trajectories on river biogeochemistry. We are continuing to monitor biogeochemical impacts within the 2020 Holiday Farm Fire throughout the recovery process, in collaboration with external partners (Cavaiani et al., in prep). We have recently begun a new collaboration with University of Idaho to study C and P chemistry before, during, and after a prescribed burn at a long-term research watershed (Reynold's Creek experimental watershed). We have also conducted a meta-analysis that considered over 174 published scientific manuscripts and found that the main detectable environmental controls on dissolved PyC (dPyC)

[1] https://data.ess-dive.lbl.gov/view/doi:10.15485/1894135

transport are the formation conditions and quality of the PyC itself, with longer and higher temperature charring conditions leading to less soluble transport of PyC, although solubility increases with increasing decomposition (Abney et al., in prep). These efforts complement the burn severity laboratory experiments detailed above; for example we see similarly see decreases in PyC mobility with increasing burn severity in our experimental leachates.

RC-3 is partnering with RC-2 FY22's spatial study to analyze the results of the in situ O_2 rates across fire- and non-fire-impacted sites in the spatial study. This analysis provided information on respiration rates in fire-impacted vs. non-fire-impacted sites during baseflow, and informed fieldwork completed in FY23. We designed and implemented a spatiotemporal study in the YRB from the Schneider Spring Fire to further improve model predictive capacity of river respiration in watersheds impacted by fire disturbances. The fieldwork completed in spring/summer 2023 captured fire-impacted and non-fire-impacted sites with similar distribution of land cover/use, slope, stream order, catchment area and discharge during periods of high hydrologic connectivity with the landscape. Based on RC-2's work, water column respiration is a trivial component of river corridor ecosystem respiration at base flow in the YRB. Visible difference in turbidity between the fire and non-fire-impacted sites during snow melt in FY23 motivated new hypothesizes on the importance of turbidity post-fire on water column respiration rates. Therefore, we hypothesize that this dynamic may shift during periods of high hydrologic connectivity (i.e., storms, snowmelt) in fire-impacted streams.

Incorporate wildfire dynamics into predictive models. In FY23, RC-1 and RC-3 formed a wildfire modeling working group to focus on wildfire impacts in watersheds. This working group focuses on linking experimental and observational data with models, deepening our conceptual understanding of different models used by the RC-SFA to study wildfires, investigating the parametrizations and key data needs supporting those models, and developing new model-generated hypotheses.

Work led by RC-3, in partnership with Oregon State University, using Wenas Creek as a test watershed, manipulates watershed parameters in the SWAT model necessary to trigger an in-stream response in biogeochemical parameters. We have identified thresholds of watershed characteristics that impact important biogeochemical parameters (total suspended solids, dissolved nitrate, dissolved organic carbon) through our model manipulations, and are comparing these model predictions to a meta-analysis of fire impacts on these parameters (Scheibe et al., in prep). Our model simulations suggest that an area burned of ~30% at moderate or high severity is necessary to see increases in total suspended solids and dissolved nitrate concentrations. These results complement ATS model predictions of no major changes in biogeochemical dynamics simulated post-fire in Wenas Creek from RC-1.

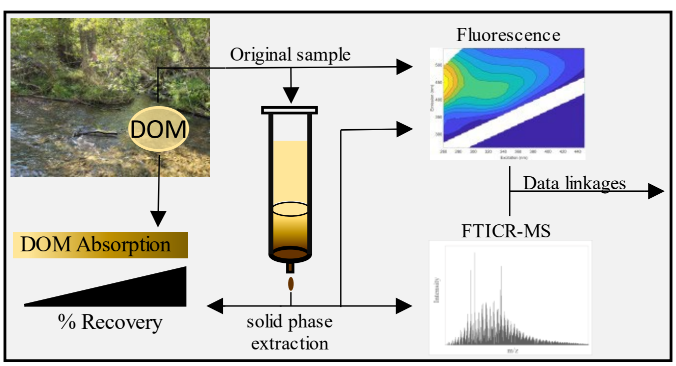

Figure 5 Conceptual flow chart highlighting linkages between the recovery of DOC from solid phase extraction with DOM light absorption and a workflow to couple optical data with ultra-high resolution mass spectrometry data.

Publication Highlight: Investigating the impacts of solid phase extraction on dissolved organic matter optical signatures and the pairing with high-resolution mass spectrometry data.

The study of DOM is integral to understanding the transport of carbon in aquatic systems. There are many techniques to study DOM and broad interest from the community to pair data streams across multiple analytical platforms, particularly those from optical and high- resolution mass spectrometry (HRMS). Recent studies have directly called into question the feasibility of pairing optical and HRMS data due to potential biases introduced by solid phase extraction as a sample preparation technique for HRMS compared to optics performed on the original sample. In this study, we directly address this concern and show that optical and HRMS datasets can still be paired despite some biases in the optical data that may result out of SPE. This work makes a key step forward in the use of optical data as surrogates for HRMS data, highlighting potential for future field-based applications and increasing our predictive understanding of DOM cycling in aquatic systems.

Reference: Roebuck, J.A., Jr., A.N. Myers-Pigg, V. Garayburu-Caruso, J. Stegen. "Investigating the impacts of solid phase extraction on dissolved organic matter optical signatures and the pairing with high-resolution mass spectrometry data." In review. *Limnology and Oceanography: Methods*.

Plans for FY24: (1) Continue to publish data packages on ESS-DIVE using reporting formats as early as possible in the research life cycle. (2) Develop a new conceptual model/hypotheses for river corridor biogeochemistry post-fire, based on model-generated hypotheses from ATS and SWAT models and data collected in ongoing field and lab efforts. (3) Complete numerous publications, summarized above, based on ongoing field and lab efforts. (4) Conduct targeted laboratory experiments focused on mechanistically understanding hot spots of sediment respiration in fire-impacted systems. These will be based on model-hypotheses generated using burn severity laboratory experiment results, with an emphasis on biogeochemical reactivity, and provide outcomes to RC-1 and MM for inclusion in mechanistic models. (5) If additional end-of-year funds are received, we will collaborate with RC-4 to expand our research efforts on fire impacts on river respiration from the reach scale to across the CONUS in both sediments and waters, using the ICON-ModEx approach.

Research Campaign 4 (RC-4): Multi-Basin Studies

Overall Objectives: *The Multi-Basin Studies Campaign aims to provide transferable principles that integrate DOM chemistry, microbial gene expression, biogeochemical function, and disturbance by combining existing global-scale data with WHONDRS-based data generation and numerical modeling distributed across CONUS basins.*

- Expand WHONDRS: Continue to develop WHONDRS as a resource to pursue community-based data analysis, interpretation, and publishing (FY21–24).
- Inform models: Couple DOM chemistry, microbial gene expression, and aerobic respiration in surface and pore water across globally distributed river corridors to inform models in RC-1,2,3 (FY21-24).
- Compare to predictions: Implement ICON-ModEx via crowdsourced sampling designed to test model predictions across CONUS basins and use outcomes to inform further model development (FY22-24).

Key Contributions of this Research Campaign to the SFA: The RCSFA aims to develop predictive capabilities and a fundamental understanding of river corridor hydrobiogeochemistry that apply across basins. This is vital to informing large-scale models that span diverse basins within and beyond CONUS. RC-4 is a key element of this long-term vision by developing transferable knowledge and models. Much of the scientific focus in RC-4 builds from RC-1,2,3 while making more direct use of WHONDRS and expanding the community-based research model that WHONDRS embodies. RC-4 is making use of existing WHONDRS data and growing WHONDRS as a community resource. For example, RC-4 has significantly expanded the WHONDRS consortium to generate transferable understanding and predictive capacity of sediment respiration across the CONUS. Through an SBIR collaboration, this work is laying the foundation for self-guided (i.e., AI-guided) river corridor science across the CONUS. In addition, RC-4-generated data are being used by RC3 to contextual PyOM chemistry against a backdrop of natural OM. RC-4 is also engaged in crowdsourced sampling campaigns around the globe to generate transferable understanding of factors governing variation in OM chemistry and the biogeochemical impacts of that variation, ultimately to inform the RCSFA's mechanistic and AI models.

FY23 Science Plan Milestone (Revised): The FY23 milestone has been revised due to a strong (though not exclusive) focus on the 'ICON-ModEx' effort, which was not envisioned when the science plan was written, as well as DOM scaling results from RC2 that inspired CONUS and multi-continent evaluations of transferability. Continue WHONDRS-based sampling, with an emphasis on understanding and predicting sediment respiration across CONUS. Build the foundation for a 'self-driving' approach to generating transferable knowledge via tight integration of ICON, ModEx, and AI at the CONUS scale. Complete analysis, using WHONDRS data across CONUS basins, of multiscale characterization of DOM chemistry. Quantify CONUS-wide linkages between DOM chemistry and microbial gene expression. Initiate international collaboration to extend evaluation of transferability of DOM scaling across North and South America.

Progress Brief for FY23: Our activities in FY23 are focused primarily on generating transferable knowledge and mutually beneficial outcomes focused on sediment respiration rates, organic matter chemistry, and microbial genomics.

ICON-ModEx: Integrating crowdsourcing, AI/ML, and remote sensing to predict sediment respiration across the CONUS. This effort, the largest RC-4 emphasis in FY23, has included monthly ModEx cycles to test and rebuild ML models followed by AI-guided weekly crowdsourced sampling across CONUS; activities for enhancing mutual benefit with stakeholders including virtual classroom presentations and an open update call; a workshop launching a crowdsourced manuscript; collaborative sampling with RC-2; and follow-on study co-design with RC-3. Two manuscripts describing the motivation, approach and results are in preparation.

ICON-based community science: We expanded the reach of the ICON Science Cooperative to support ICON science within and outside of the SFA. This has included developing design resources for projects to use at any phase of the research life cycle; collaborating on university proposals to integrate WHONDRS and ICON; providing assistance to other teams learning to use ESS-DIVE Reporting Formats; and engaging with researchers across disciplines to understand the challenges and opportunities for ICON to increase transferability and mutual benefit more broadly. We facilitated a series of crowdsourced manuscripts based on WHONDRS data to deepen understanding of OM dynamics and mechanistic linkages between microbial respiration and OM thermodynamics, stoichiometry, and molecular size. One paper in the collection (Stadler et al., 2023) found that that core DOM compounds, present in many river systems, had consistent molecular properties, while satellite compounds varied widely. Core compounds exhibited molecular characteristics that suggest higher persistence in the environment. The findings point to the use of data-driven approaches to separate rare and common compounds to reduce DOM complexity. Another paper (Ahamed et al. 2023) used ML to discover the pool of bioavailable organic molecules that explain variation in sediment respiration rates across CONUS. These molecules have distinct chemistry relative to other organic molecules from riverbed sediments. The resulting knowledge will enable critical next steps in transferable, process-based predictions of river corridor biogeochemistry. We are major contributors to the development, use, and publication of the Genome-Resolved Open Watersheds (GROW) database, which is a community resource led by Kelly Wrighton to enable multi-omics analyses of global river corridors. The first GROW manuscript (Borton et al., in prep) will be submitted in July, focused on revealing mechanisms of carbon cycling in rivers. GROW has become a key use case for the integration of BER capabilities, including EMSL, JGI, NMDC, ESS-DIVE, and KBase. We also co-designed and began implementing international collaborations spanning South American ecoregions and Svalbard, Norway, facilitating (1) the SFA's ability to test transferability of patterns observed in the YRB to generate knowledge that is relevant across global rivers and (2) value for the collaborators in a mutually beneficial way. Finally, we rapidly (i.e., before data use/analysis) published FAIR (meta)data on ESS-DIVE using ESS-DIVE Reporting Formats, including new data packages[1] and adding new data to pre-existing data packages[2]. These datasets include CONUS-scale studies, localized stream or watershed-specific studies, and more than 20 different data types, and they require optimizing strategies to meet the needs for rapid data access and for high-quality FAIR data.

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[1] https://data.ess-dive.lbl.gov/view/doi:10.15485/1969114; https://data.ess-dive.lbl.gov/view/doi:10.15485/1888571; https://data.ess-dive.lbl.gov/view/doi:10.15485/1895159; https://data.ess-dive.lbl.gov/view/doi:10.15485/1898913; https://data.ess-dive.lbl.gov/view/doi:10.15485/1923689

[2] https://data.ess-dive.lbl.gov/view/doi:10.15485/1603775; https://data.ess-dive.lbl.gov/view/doi:10.15485/1729719

Analyses of WHONDRS data identify OM and microbial drivers of river corridor biogeochemistry: We conducted a metanalysis using time-resolved WHONDRS data from seven globally distributed rivers. We combined DOM characterization, geochemical analysis, and shotgun metagenomic sequencing with ecological analyses to assess environmental interactions that could explain global river corridor DOM variation. These analyses revealed that global variation of DOM composition in river corridors is primarily shaped by environmental factors (geochemical and lithological conditions), with globally distributed microbial species showing consistent roles in carbon degradation.

We completed a multi-omics analysis of sediments to understand fundamental mechanisms through which bacteria and viruses jointly couple carbon and nitrogen cycles within the hyporheic zone (Rodríguez-Ramos et al., 2022). Based on an integrated data set of 33 metagenomes, metaproteomes, and paired metabolomes, we reconstructed >500 microbial metagenome-assembled genomes (MAGs) and 111 viral MAGs (vMAGs). We uncovered new roles for microorganisms in organic matter decomposition, carbon sequestration, and nitrogen cycling. These metabolic pathways are integrated through shared resource pools of ammonium, carbon dioxide, and inorganic nitrogen, and contribute to greenhouse gas production from hyporheic sediments. Further, we linked vMAGs to MAGs to provide some of the first insights into viral modulation of river sediment carbon and nitrogen cycling. Subsequently, we reconstructed 6,500 viral and 1,033 microbial genomes and found distinct communities associated with surface and pore water environments within a river corridor sampled by WHONDRS every 3 hours over 48 hours (Rodríguez-Ramos et al., in review). About 70% of the viral community was persistent in surface waters, whereas only 13% was persistent in pore water. Linkages between 73 viral and 38 microbial genomes were found and indicate that viruses are key contributors to carbon and nitrogen cycling in rivers. The results together show that microbial and viral communities can exist as stable communities in river corridors with strong interactions between them that impact biogeochemical cycles.

We continued exploring the transferability of basin-scale DOM patterns observed in the YRB (via RC-2) across multiple CONUS basins, in collaboration with Oregon State University and USGS. This effort seeks to uncover generalized patterns linked to DOM composition and transformations across five diverse basins, and to parse out the influences of drainage area and land use patterns. The results will identify transferable principles that can be implemented in mechanistic models to improve predictions of river corridor biogeochemistry. We also investigated the hypothesis that sediment metal content will help explain the longitudinal structuring of OM composition released from HZ sediments at the CONUS scale. This study used WHONDRS field campaign data including DOM chemistry (FTICR-MS) and mineral elemental data (XRF), augmented with USGS soil elemental data and landcover data. We discovered weak relationships between hyporheic zone pore water DOM compound composition and mineral elemental Cu at the CONUS scale but not with Fe, suggesting that linkages of Fe-DOM may be strong at site to regional scales and less so at the continental scale. Finally, we developed and tested new models of drivers of hyporheic zone respiration. Leveraging numerical experiments, we found that variations in microbial biomass provided additional explanatory power for the observed distribution of rate measurements among 250 individual locations within WHONDRS network. Additionally, we found that microbially accessible OM was significantly lower than bulk measurements, which explained the constraining boundary of observed respiration rates (Figure 6). This exercise illustrated the concept and application of hypothesis-driven ModEx, which focuses on iteratively generating and testing hypotheses. Follow-up experiments should focus on manipulating OM accessibility at batch scale and identifying proxy measurements for OM accessibility at field scale.

Publication Highlight: Maximum Respiration Rates in Hyporheic Zone Sediments are Primarily Constrained by Organic Carbon Concentration and Secondarily by Organic Matter Chemistry: Rivers are fundamental components of the Earth system, and their biogeochemistry can be heavily influenced by processes in subsurface zones immediately below the riverbed, referred to as the hyporheic zone. Within the hyporheic zone, OM fuels microbial respiration, and OM chemistry heavily influences aerobic and anaerobic biogeochemical processes. The link between OM chemistry and respiration has been hypothesized to be mediated by OM molecular diversity, whereby respiration is predicted to decrease with increasing diversity. Here we test the specific prediction that aerobic respiration rates will decrease with increases in the number of unique organic molecules (i.e., OM molecular richness, as a measure of diversity). We use publicly available data across the United States from crowdsourced samples taken by the WHONDRS consortium. Our continental-scale analyses rejected the hypothesis of a direct limitation of respiration by OM molecular richness. In turn, we found that OC concentration imposes a primary constraint over hyporheic zone respiration, with additional potential influences of OM richness. These results indicate that maximum respiration rates may be governed primarily by OC concentration, with secondary influences from OM richness. Our results also show that other variables often suppress respiration rates below the maximum associated with the richness-to-concentration ratio (**Figure 6**). An important focus of future research will identify physical (e.g., sediment grain size), chemical (e.g., nutrient concentrations), and/or biological (e.g., microbial biomass) factors that suppress hyporheic zone respiration below the constraint boundaries observed here.

Citation: Stegen, James C., Vanessa A. Garayburu-Caruso, Robert E. Danczak, Amy E. Goldman, Lupita Renteria, Joshua M. Torgeson, and Jacqueline R. Wells. "Hyporheic Zone Respiration Is Jointly Constrained by Organic Carbon Concentration and Molecular Richness." Accepted for publication in *Biogeosciences*. Preprint: *EGUsphere*, August 1, 2022, 1–15. https://doi.org/10.5194/egusphere-2022-613.

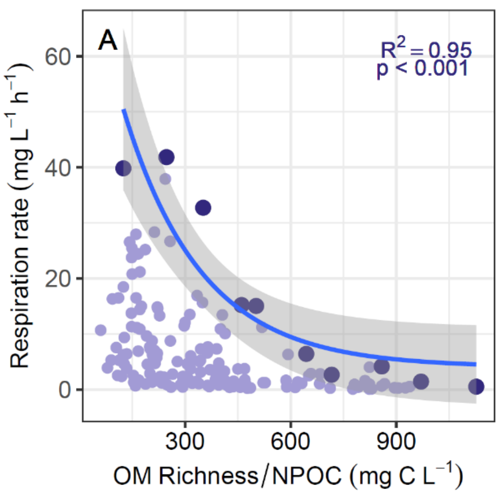

Figure 6 Across CONUS, maximum sediment respiration rate decreased with increasing values for the ratio of OM molecular richness to non-purgeable organic carbon concentration (NPOC). This is a transferable relationship across diverse river systems and is part of hypothesis-driven ModEx cycles pursued by the MM activity (see below). Maximum respiration rates (shown in the darker colors) were found by subdividing each horizontal axis into 10 even bins. All other respiration rates and the corresponding richness-to-concentration ratios are shown in lighter colors. Solid lines represent negative exponential models fit to the maximum respiration rates, with shaded areas indicating 95% confidence intervals. Statistics for each model are provided on each panel.

Plans for FY24: (1) Continue to publish data packages on ESS-DIVE using reporting formats as early as possible in the research life cycle. (2) Collaborate with Parallel Works to complete analyses and associated manuscripts from the ICON-ModEx effort. (3) Complete CONUS-wide evaluation of transferability in DOM scaling observed at the basin scale in RC-2, and continue pursuing evaluation of DOM scaling across South America. (4) Evaluate the degree of coordination between scaling of microbial functional diversity and scaling of DOM biochemical transformation diversity in water and sediment across CONUS. (5) Complete ModEx-based collaboration with MM focused on understanding factors that suppress sediment respiration below the maximum constraint boundary imposed by the ratio of OM richness-to-organic C concentration. (6) Facilitate completion of crowdsourced manuscripts focused on analysis of previously published WHONDRS data. (7) Pursue additional sequencing of sediment microbial communities, ultrahigh resolution characterization of OM chemistry, and other molecular analyses collected during the ICON-ModEx effort to enable evaluation of the ML model performance with and without molecular data. (8) Develop additional resources to facilitate broader use of ICON science across the RCSFA, the ESS science community, and beyond. (9) If additional end-of-year funds are received, we will build from the ICON-ModEx effort in collaboration with RC-3 to characterize, understand, and predict impacts of fire on respiration in sediments and water across the CONUS.

<u>Multiscale ModEx:</u>

Overall Objectives: *The MM cross-cutting activity aims to coordinate model–data integration across RCs and scales, assuring optimal use of data and models and open distribution of SFA products.*

- Steward interactive data–model integration (ModEx) across scales and all RCs.
- Implement the Data Management Plan (DMP) and Software Productivity and Sustainability Plan (SW-PSP); provide tools for accessing data and software products.

Progress Brief for FY23: The MM activity does not have specific milestones. In FY23, the MM cross-cutting activity solicited proposals from SFA early career staff members for integrative tasks in collaboration with one or more Research Campaigns. Two such activities have been funded and are underway:

1. <u>Improving Mechanistic Modeling of Hyporheic Zone Biogeochemistry</u> (Lead: Jianqiu Zheng) This effort, collaborative with RC-2 and RC-4, builds on observed variations in hyporheic zone sediment respiration rates (Figure 6). Thermodynamic modeling based on prior SFA research are being used to test new hypotheses regarding the sources of the observed variation (specifically substrate availability and microbial biomass) and generate new hypotheses that can be tested empirically, following a hypothesis-driven ModEx approach. Dr. Zheng presented this work in a poster at the 2023 ESS PI Meeting.
2. <u>Upscaling Streambed Sediment-Flux-Respiration Interactions from Sediment to Watershed Scale using Multiscale ModEx</u> (Lead: Yunxiang Chen) This effort, in collaboration with RC-1 and RC-2, is developing cellphone- and drone-based photogrammetry and AI methods for quantifying riverbed grain size distributions in the field, extrapolating 3D riverbed structure from 2D images, and simulating hydrologic exchange across multiple physical scales. Preliminary results were presented to program managers by Dr. Chen at our May monthly meeting (May 24, 2023)

The River Corridor SFA has a dedicated data management (DM) team funded under the MM activity to support the entire project in implementing our DMP, which adheres to the SC and BER data management requirements. The DM team has established standardized processes (requirements and recommendations) consistent with the DMP that are followed by all RCs. DM team members support individual researchers in creation of data packages associated with publications and/or data collection campaigns and their open publication on the ESS-DIVE repository. All data packages follow the community reporting formats developed by ESS-DIVE with the ESS community.

Publication Analysis

103 peer-reviewed journal articles and one book chapter have been published during the current performance period (2020 through current date - see Appendix A for a complete list). Additionally, five journal articles have been accepted and 23 manuscripts have been submitted as of the writing of this document. As shown in Figure 7, the total number of publications in the three-year period 2020-2022 exceeds that of the prior triennial period (2017-2019) by more than twenty papers and is an even greater increase relative to the triennial period 2014-2016. Over the current period, the SFA published most frequently in *Water Resources Research* (12 papers) and *Frontiers in Water* (9 papers). Outside of these two journals, the remaining papers were published in 56 different journals, reflecting the diversity of SFA research and the wide audience reached by our publications. The SFA publishes in high-quality journals: Five publications are in DOE-designated high-impact journals (one in *Nature*, one in *Nature Biotechnology*, one in *Nature Microbiology*, and two in *Nature Communications*), 40% of the publications are in ISI-designated top ten journals in their respective fields, more than 70% are in first quartile journals, and nearly all (98%) are in journals with impact factors above the median in their field. The average impact factor of the journals for which data are available (weighted by the number of SFA papers published in each) is 8.15, a 22% increase from the value of 6.89 reported in 2021.

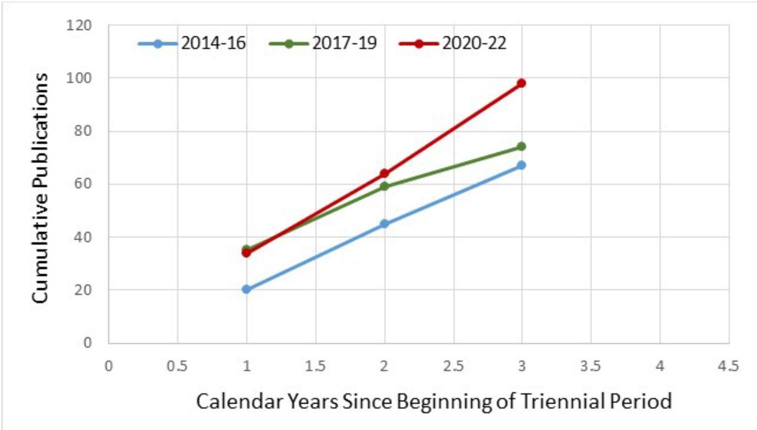

Figure 7. Comparison of the number of publications to date in the most recent three-year period (2020-2022) with the number of publications in the two previous triennial periods (2014-16 and 2017-19).

In addition to peer-reviewed written publications, the SFA places high value on the publication of high-quality data packages on the ESS-DIVE repository. The project maintains two data portals on ESS-DIVE[1], one for general SFA data packages and a second specifically for WHONDRS data. As of the writing of this document, the SFA has published 36 data packages linked to the SFA project portal. The WHONDRS portal contains 22 data packages including many that are also linked to the SFA portal as well as others from related projects (e.g., Stegen Early Career Project). These data packages include observational data from a variety of field campaigns, model data from simulations, and data related to specific literature publications. We follow ESS-DIVE community reporting formats to ensure high-quality, FAIR data that is useful to and usable by the community.

Future Scientific Goals, Vision, and Plans for Meeting Program Objectives

The Environmental System Science program examines complex ecological and hydro-biogeochemical processes within terrestrial and coastal systems to understand inherent and emergent properties of changes to Earth and environmental systems.[2] The long-term vision of the SFA, closely aligned with ESS objectives, will culminate in transferable understanding of critical hydrologic, biogeochemical, and ecological processes in river corridors, and in the creation of a new broadly applicable simulation capabilities, linked with other watershed hydrobiogeochemical system component models, to provide predictive understanding of watershed function and response to disturbances. In the current performance period (FY21-24), we have expanded our research to study the YRB, which encompasses a broad range of physiographic and hydrobiogeochemical environments. We continue to strengthen our broad collaborations, e.g., through WHONDRS and other efforts, to support generalization of new knowledge, as embodied in numerical models, across the CRB and the CONUS, and integration of those models with major community Earth system model frameworks such as E3SM.

New Scientific Results that may Shift Current Research or Motivating Knowledge Gaps

FY23 is the third year of the current performance period for which our research plan was reviewed in 2020. The plan is currently being implemented largely as written, with the exceptions of 1) modifications to RC3 and RC4 made in response to reviewer comments and BER guidance[3]; 2) modifications to the RC2 FY23 milestone as described above; and 3) modifications to the RC4 FY23 milestone as described above. The project performance period was extended one year (through FY24) in accommodation for COVID-related delays and challenges. No near-term major changes in direction or activity plans have been identified at the current time. We conducted a stocktaking meeting in February 2023 to develop

[1] https://data.ess-dive.lbl.gov/portals/PNNLRiverCorridorSFA; https://data.ess-dive.lbl.gov/portals/WHONDRS
[2] https://ess.science.energy.gov/
[3] PNNL SBR SFA Reponses to the Triennial Review Comments, Transmitted to BER October 12, 2020.

more detailed plans and timeline for FY23-24 and initiate planning for the new Science Plan to be submitted in early CY2024. Based on that meeting and results to date, we will continue to focus our research in the YRB, with the exception of RC-4 which incorporates the WHONDRS and ICON-MODEX efforts. An emerging scientific theme is the role of non-perennial streams in watershed hydrobiogeochemical cycling. For example, one of our fire-impacted sites in the YRB (Wenas Creek) is normally hydrologically disconnected from the terrestrial landscape due to its arid nature. However, in 2022 we observed significant flow in intermittent tributaries that interacted strongly with the burned regions. Non-perennial streams are one type of variably inundated environment (others include coastal systems, vernal ponds, floodplains, and wetlands). In previous SFA research (Goldman et al., 2017; Song et al., 2021), we have studied the impacts of temporally variable inundation cycles in river parafluvial zones; this research interest is expanding toward other variably inundated watershed subsystems. The SFA led the Variably Inundated Environments Workshop on May 4–5, 2022 with co-leaders Daniel Allen (Penn State Univ.) and Amy Burgin (Univ. of Kansas). The workshop was attended by approximately 40 persons from the research community and we are currently engaging with the participants to develop and submit a manuscript based on the workshop outcomes.

Collaborative Research Activities

The SFA is dedicated to implementing ICON science principles as an integrated and collaborative team (DOE, 2019). We have dramatically increased our collaborative footprint over the past several years through a number of avenues including (1) direct-funded (by subcontract) collaborations with universities, other national laboratories, and other federal agencies (e.g., USGS); (2) collaborative projects funded through SFA FOAs to university partners; (3) collaborative projects funded through the SBIR program; and (4) extensive community-oriented science activities. A detailed list of collaborative projects and activities with co-PI names, institutions, and titles is provided in Appendix B.

APPENDIX A: PROJECT PUBLICATIONS

2023 (as of June 30):

Published:

1. Chen K., Chen X., Stegen J. C., Villa J. A., Bohrer G., Song X., Chang K. Y., Kaufman M., Liang X., Guo Z., Roden E. E. and Zheng C. (2023). Vertical hydrologic exchange flows control methane emissions from riverbed sediments. *Environmental Science & Technology* **57**(9), 4014-4026; doi: 10.1021/acs.est.2c07676.
2. Fulton S., Stegen J. C., Kaufman M. H., Thompson A. and Dowd J. (2023) Laboratory evaluation of open source and commercial electrical conductivity sensor precision and accuracy: How do they compare? *PLoS One*, 18(5): e0285092, doi: 10.1371/journal.pone.0285092.
3. McDowell N. G., Anderson-Teixeira K., Biederman J. A., Breshears D. D., Fang Y., Fernández-de-Uña L., Graham E. B., Mackay D. S., McDonnell J. J., Moore G. W., Nehemy M. F., Stevens Rumann C. S., Stegen J., Tague N., Turner M. G. and Chen X. (2023). Ecohydrological decoupling under changing disturbances and climate. *One Earth* **6**(3), 251-266; doi: https://doi.org/10.1016/j.oneear.2023.02.007.
4. Moreland K. C., Barnes M. E., O'Geen A., Dove N., Hart S. C. and Berhe A. A. (2023). Climatic controls on soil and saprock nitrogen distribution and persistence in the Sierra Nevada. *Journal of Plant Nutrition and Soil Science* **186**(1), 116-129; doi: 10.1002/jpln.202200218.
5. Xiao Y., Sloan J., Hepworth C., Fradera-Soler M., Mathers A., Thorley R., Baillie A., Jones H., Chang T., Chen X., Yaapar N., Osborne C. P., Sturrock C., Mooney S. J., Fleming A. J. and Zhu X. G. (2023). Defining the scope for altering rice leaf anatomy to improve photosynthesis: a modelling approach. *New Phytol* **237**(2), 441-453; doi: 10.1111/nph.18564.

Accepted:

1. Ahamed F., You Y., Burgin A., Stegen J. C., Scheibe T. and Song H.-S. (2023). Exploring the determinants of organic matter bioavailability through substrate-explicit modeling. *Frontiers in Water*, Accepted, doi: 10.3389/frwa.2023.1169701.
2. Danczak R., Garayburu-Caruso V. A., Renteria, L., McKever S., Otenburg O., Grieger S. R., Son K., Kaufman M., Fulton, S. G., Roebuck J. A., Myers-Pigg A. and Stegen J. C. (2023). Riverine organic matter functional diversity increases with catchment size. *Frontiers in Water*, Accepted, doi: 10.3389/frwa.2023.1087108
3. Graham E., Song H., Grieger S., Garayburu-Caruso V., Stegen J. C., Bladon K. D. and Myers-Pigg A. (2023). Potential bioavailability of representative pyrogenic organic matter compounds in comparison to natural dissolved organic matter pools. *EGUsphere*, Accepted; MS# egusphere-2022-2194.
4. Song H., Grieger S., Garayburu-Caruso V., Stegen J. C., Bladon K. D. and Myers-Pigg A. (2023). Potential bioavailability of representative pyrogenic organic matter compounds in comparison to natural dissolved organic matter pools. *EGUsphere*, Accepted; MS# egusphere-2022-2194.
5. Stadler M., Barnard M., Bice K., De Melo M., Dwivedi D., Freeman E., Garayburu-Caruso V., Linkhorst A., Mateus-Barros E., Shi C., Tanentzap A. and Meile C. (2023). Applying the core-satellite species concept: Characteristics of rare and 2 common riverine dissolved organic matter. *Frontiers in Water*, Accepted, doi: 10.3389/frwa.2023.1156042.

Submitted:

1. Bao Y., Feng Y., Stegen J., Wu M., Chen R., Liu W., Zhang J., Li Z. and Lin X. (2023) Integrating assembly processes, community patterns, and ecosystem function in the context of organic matter degradation. *Nature Ecology & Evolution*, Submitted; 6.13.19.

2. Chen S., Garayburu-Caruso V., Stegen J. C., Goldman A., Lu M. and Lu Y. (2023). Changes of dissolved organic matter source and lability in relation to stream metabolism along a fluvial continuum section of a subtropical river. *Water Research*, Submitted; MS# WR-S-23-01863.
3. Chen K., Yang S., Roden E., Chen X., Chang K. Y., Guo Z., Liang X., Ma E., Fan L. and Zheng C. (2023). Influence of vertical hydrologic exchange flow, channel flow and biogeochemical kinetics on CH4 emissions from rivers. *Water Resources Research*, Submitted.
4. Gomez-Velez J. D., Cardenas M. B., Chen X. and Scheibe T. D. (2023) Riverbed respiration produces a globally significant amount of CO2. *Nature*, Submitted; 2020-09-17406.
5. Hou Z., Ray J., Huang M., Bao J., Ren H. and Swiler L. (2023) Machine learning-based feature selection and surrogate-based MCMC-bayesian inversion for improving runoff simulations in the community land model. *Water Resources Research*, In revision.
6. Hu H., Leung L. R., Dominguez F., Gochis D., Chen X., Good S., Dugger A., Larsen L. and Barlage M. (2023). Effect of Lateral Flow on Transit Times: integrating a water tracer model to WRF-Hydro. *Water Resources Research*, Submitted.
7. Kang Y., Homer M., Gladwin E., de Clerck A., Jones N., Ruan H., Garayburu-Caruso V., Resch C. and Stegen J. C. (2023). Selective and sensitive determination of Mn(II) by cathodic stripping voltammetry with integrated microelectrode-based sensor chips. *Journal of Electroanalytical Chemistry*, Submitted; MS# JELECHEM-D-23-00273.
8. Karra S., Apte S. V., He X. and Scheibe T. (2023) Pore-resolved simulations of turbulent boundary layer flow over permeable and impermeable sediment beds. *Journal of Fluid Mechanics*, Submitted.
9. Karra S., Admmed B. and Mudunuru M. (2023) AdjointNet: Constraining machine learning models with physics-based codes. *Journal of Computational Physics*, Submitted.
10. Kaufman M., Torgeson J. M. and Stegen J. C. (2023). Metabolic Multireactor: practical considerations for using simple oxygen sensing optodes for high-throughput batch reactor metabolism experiments. *Plos One*, Submitted; MS# PONE-D-23-06927.
11. Li B., Cardenas M. B., Chen X. and Liu X. (2023) Mechanistic definition and prediction of the mass transfer coefficient between rivers and hyporheic zones: the a of two Ωs. *Water Resources Research*, Submitted.
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13. Perez Mesa G., Gomez-Velez J., Chen X. and Scheibe T. (2023). The directional unit hydrograph method: Connecting streamflow response to storm dynamics. *Journal of Hydrology*, Submitted.
14. Rodriguez-Ramos J., Oliverio A., Borton M. A., Mueller B. M., Schulz H., Flynn R. M., Daly R. A., Danczak R., Ellenbogen J., Schopflin L., Shaffer M., Goldman A., Lewandowski J., Stegen J. C., and Wrighton K. C. (2023) Spatial and temporal metagenomics of river compartments reveals viral community dynamics in an urban impacted stream. *Frontiers in Microbiomes*, Submitted
15. Roebuck J., Myers-Pigg A., Garayburu-Caruso V. and Stegen J. C. (2023). Investigating the impacts of solid phase extraction on dissolved organic matter optical signatures and the pairing with high-resolution mass spectrometry data. *Limnology and Oceanography Methods*, Submitted.
16. Roley S., Hall B., Perkins W., Garayburu-Caruso V. and Stegen J. C. (2023). High rates of ecosystem metabolism in the Hanford Reach of the Columbia River. *Limnology and Oceanography*, Submitted; MS# LO-23-0122.
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20. Shuai P., Chen X., Hammond G., Song X., Chen K. and Zachara J. (2023) Hydrologic exchange flows alter river corridor thermal regimes in a dam-regulated river. *Water Resources Research*, Submitted 10/19; 2019WR026459.
21. Shuai P., Jiang P., Coon E. and Chen X. (2023). The importance of explicitly representing the streambed in watershed models. *Hydrological Processes*, Submitted; MS# HYP-23-0224.
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3. Arora B., Briggs M., Zarnetske J., Stegen J. C., Gomez-Velez J., Dwivedi D. and Steefel C. (2022). Hot Spots and Hot Moments in the Critical Zone: Identification of and Incorporation into Reactive Transport Models. *In* Biogeochemistry of the Critical Zone: Advances in Critical Zone Science. A. S. Wymore, W. H. Yang, W. L. Silver, W. H. McDowell and J. Chorover, Eds., Springer-Nature. doi: 10.1007/978-3-030-95921-0_2.
4. Bao J., Chen Y., Fang Y., Song X., Perkins W., Duan Z., Shuai P., Ren H., Hou Z., Richmond M., He X. and Scheibe T. (2022) Modeling framework for evaluating the impacts of hydrodynamic pressure on hydrologic exchange fluxes and residence time for a large-scale river section over a long-term period. *Environmental Modelling & Software*, **148**, 105277; doi: 10.1016/j.envsoft.2021.105277.
5. Borton M. A., Collins S. M., Graham E. B., Garayburu-Caruso V. A., Goldman A. E., de Melo M., Renteria L., Stegen J. C. and W. C. C. (2022) It takes a village: Using a crowdsourced approach to investigate organic matter composition in global rivers through the lens of ecological theory. *Frontiers in Water*, **4**, 870453; doi: 10.3389/frwa.2022.870453.
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Scheibe T. D., Wainwright H. M., Williams K. H. and Zavarin M. (2022) From legacy contamination to watershed systems science: A review of scientific insights and technologies developed through DOE-supported research in water and energy security. Environmental Research Letters, 17, 043004; doi: 10.1088/1748-9326/ac59a9.

9. Fremin B. J.Bhatt A. S.Kyrpides N. C.Sengupta A.Sczyrba A.Maria da Silva A.Buchan A.Gaudin A.Brune A.Hirsch A. M.Neumann A.Shade A.Visel A.Campbell B.Baker B.Hedlund B. P.Crump B. C.Currie C.Kelly C.Craft C.Hazard C.Francis C.Schadt C. W.Averill C.Mobilian C.Buckley D.Hunt D.Noguera D.Beck D.Valentine D. L.Walsh D.Sumner D.Lymperopoulou D.Bhaya D.Bryant D. A.Morrison E.Brodie E.Young E.Lilleskov E.Högfors-Rönnholm E.Chen F.Stewart F.Nicol G. W.Teeling H.Beller H. R.Dionisi H.Liao H.-L.Beman J. M.Stegen J.Tiedje J.Jansson J.VanderGheynst J.Norton J.Dangl J.Blanchard J.Bowen J.Macalady J.Pett-Ridge J.Rich J.Payet J. P.Gladden J. D.Raff J. D.Klassen J. L.Tarn J.Neufeld J.Gravuer K.Hofmockel K.Chen K.-H.Konstantinidis K.DeAngelis K. M.Partida-Martinez L. P.Meredith L.Chistoserdova L.Moran M. A.Scarborough M.Schrenk M.Sullivan M.David M.O'Malley M. A.Medina M.Habteselassie M.Ward N. D.Pietrasiak N.Mason O. U.Sorensen P. O.Estrada de los Santos P.Baldrian P.McKay R. M.Simister R.Stepanauskas R.Neumann R.Malmstrom R.Cavicchioli R.Kelly R.Hatzenpichler R.Stocker R.Cattolico R. A.Ziels R.Vilgalys R.Blumer-Schuette S., et al. (2022) Thousands of small, novel genes predicted in global phage genomes. *Cell Reports*, **39**, 110984; doi: https://doi.org/10.1016/j.celrep.2022.110984.
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11. Hills D. J., Damerow J. E., Ahmmed B., Catolico N., Chakraborty S., Coward C. M., Crystal-Ornelas R., Duncan W. D., Goparaju L. N., Lin C., Liu Z., Mudunuru M. K., Rao Y., Rovetto R. J., Sun Z., Whitehead B. P., Wyborn L. and Yao T. (2022) Earth and Space Science Informatics Perspectives on Integrated, Coordinated, Open, Networked (ICON) Science. *Earth and Space Science*, **9**, e2021EA002108; doi: 10.1029/2021ea002108.
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16. Kaufman M. H., Ghosh R., Grate J., Shooltz D., Freeman J., Ball T., Loloee R., McIntire C., Wells J., Strickland C., Vermeul V. R., Rod K. A., Mackley R. D., Lin X., Ren H. and Stegen J. (2022) Dissolved oxygen sensor in an automated hyporheic sampling system reveals biogeochemical dynamics. *PLOS Water* 1(4): e0000014, doi: 10.1371/journal.pwat.0000014.
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20. Mudunuru M. K., Son K., Jiang P., Hammond G. and Chen X. (2022). Scalable deep learning for watershed model calibration. F*rontiers in Earth Science* **10**, doi: 10.3389/feart.2022.1026479.
21. Nelson A. R., Toyoda J., Chu R. K., Tolić N., Garayburu-Caruso V. A., Saup C. M., Renteria L., Wells J. R., Stegen J. C., Wilkins M. J. and Danczak R. E. (2022) Implications of sample treatment on characterization of riverine dissolved organic matter. *Environmental Science: Processes & Impacts*, **24**, 773-782; doi: 10.1039/D2EM00044J.
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23. Rodriguez-Ramos J. A., Borton M. A., McGivern B. B., Smith G. J., Solden L. M., Shaffer M., Daly R. A., Purvine S. O., Nicora C. D., Eder E. K., Lipton M., Hoyt D. W., Stegen J. C. and Wrighton K. C. (2022) Genome-resolved metaproteomics decodes the microbial and viral contributions to coupled carbon and nitrogen cycling in river sediments. *mSystems*, e0051622.
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25. Rubinstein R. L., Borton M. A., Zhou H., Shaffer M., Hoyt D. W., Stegen J., Henry C. S., Wrighton K. C. and Versteeg R. (2022) ORT: A workflow linking genome-scale metabolic models with reactive transport codes. *Bioinformatics*, **38**, 778-784; doi: 10.1093/bioinformatics/btab753.
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APPENDIX B: DETAILED LISTING OF COLLABORATIVE PROJECTS

Direct-Funded Collaborations – The SFA has directly funded the following external collaborations during FY20-23 to date (costs shown are burdened FY23 allocations):

- (2017-Current) Heping Liu, Washington State University – Install, maintain, and process data from eddy flux towers at multiple locations (RC-1, $80,122).
- (2017-2022) Jesus Gomez-Velez, Vanderbilt University – Develop and apply the NEXSS model and other analytical methods to evaluate HEFs and link to other modeling efforts (MM, $0). *Dr. Gomez-Velez moved from Vanderbilt University to ORNL during FY22 and this subcontract has been discontinued.*
- (2019-Current) Kelly Wrighton, Colorado State University – Collaborate on microbial community analysis including metagenomics studies for WHONDRS (RC-4, $19,458).
- (2019-Current) Mark Mastin, US Geological Survey – Install and maintain river water quality monitoring system and incorporate data into USGS water data system. (RC-1, $73,117)
- (2020-Current) Hyun-Seob Song, University of Nebraska Lincoln – Develop methods for integrating multi-omics data into reactive transport models, and link to other modeling efforts. (MM, $62,953)
- (2021-Current) Bob Hall, University of Montana – Collaborate on design, modeling and interpretation of riverine respiration autochamber data. (RC-2, $31,304)
- (2022-Current) Kevin Bladon, Oregon State University – Collaborate on burn severity studies and numerical modeling of wildfire watershed impacts. (RC-3, $45,784)

ESS-Funded University Collaborations – The SFA has collaborated closely with several university-led projects funded by the ESS program during FY20-23:

Co-Funded Collaborations (PNNL receives limited supplemental funds under these projects):

- (FY19-21) Bayani Cardenas (University of Texas Austin): Respiration in Hyporheic Zones: Advancing the Understanding of Coupled Transport and Microbial Biogeochemistry and their Representation in Open-source Mechanistic Models
- (FY17-20) Michael Gooseff (University of Colorado) Quantifying Distributed Exchanges of Groundwater with River Corridors
- (FY20-22) Matt Ginder-Vogel (University of Wisconsin) Particulate Organic Matter (POM) Transport and Transformation at the Terrestrial-Aquatic Interface

Unfunded Collaborations (PNNL receives no supplemental funds under these projects):

- (FY22-24) Allison Veach (University of Texas at San Antonio): Examining respiration and carbon flow in intermittent, urban rivers using novel chamber methodologies.

WHONDRS – Collaborative relationships within WHONDRS are too numerous to list.

SBIR-Funded Industrial Collaborations – The SFA works with a number of small businesses to apply and test new field, laboratory and modeling technologies. For example, we are teaming with Parallel Works, Inc. on a SBIR Phase II project "A Platform for Scientific Data Management, Modeling and Analysis with Machine Learning" in support of the ICON-ModEx effort.

Community-level Collaborations:

- 2023 ESS PI Meeting: James Stegen participated on a plenary session Early Career Panel. Allison Myers-Pigg co-led (with Michelle Newcomer, LBNL) a breakout session on "Disturbance and

Resilience." Tim Scheibe co-led (with Nicola Falco, Robinson Negron-Juarez, and Marcos Longo, LBNL) a breakout session on "Remote Sensing / AI-ML / Crowdsourcing".

- ESS Cyberinfrastructure Working Groups: Co-PI Xingyuan Chen represents the SFA on the Executive Committee and co-leads the Data–Model Integration working group, and other SFA team members participate in working group activities. Several SFA team members participated in the annual CIWG meeting the day prior to the ESS PI Meeting: Tim Scheibe gave a plenary flash talk and co-led (with Forrest Hoffman, ORNL) a breakout session on ModEX.
- ESS-Dive: The SFA has published numerous public data packages on the ESS-Dive repository in accordance with our DMP (see information in main text above).
- KBase and EMSL: SFA collaborator Hyun-Seob Song is working closely with KBase staff (Chris Henry of ANL) to develop new workflows to integrate multi-omics data into microbial community reaction networks. These networks are then formulated into elemental reaction pathways that can be incorporated into reactive transport simulations using the PFLOTRAN reaction sandbox.
- IDEAS-Watersheds: Co-PI Xingyuan Chen is the PNNL lead for the IDEAS-Watersheds collaborative project. Under this project the SFA is co-funding a postdoctoral associate working on development of community cyberinfrastructure.
- ExaSheds: Co-PI Xingyuan Chen is the PNNL lead for the ExaSheds project, which is developing next-generation high-performance watershed modeling capabilities that are integrated with and informed by artificial intelligence methodologies.
- WHONDRS Network: WHONDRS is a global consortium of researchers and other interested parties that aims to understand coupled hydrologic, biogeochemical, and microbial function, from local to global scales, within river corridors experiencing recurring, episodic, or chronic hydrologic perturbations. WHONDRS is coordinated by the SFA, and information on current activities is described above under RC-4. WHONDRS is linked with the GROW[1] network led by Kelly Wrighton (Colo. State Univ.).
- ICON Science Cooperative: James Stegen and Amy Goldman co-founded (with Sujata Emani, USDA-ARS) the Integrated Coordinated Open Networked (ICON) Science Cooperative, and WHONDRS is a partner in the Cooperative with Exchange (COMPASS-FME project) and GROW project led by Kelly Wrighton. The Cooperative is working to enable the broad use of ICON principles (founded in the ESS workshop on Open Watersheds by Design) across science sectors, to dramatically accelerate scientific progress while enhancing equity. For more information, see https://www.pnnl.gov/projects/icon-science.
- Crowdsourced Paper Collection: Kayla Borton, James Stegen, and Amy Goldman are coediting (with Sarah Collins, Univ. of Wyoming and Michaela Ladeira de Melo, University of Quebec at Montreal) a research topic in *Frontiers in Water* entitled "Crowdsourced Understanding of Global River Organic Matter Composition through the Lens of Ecological Theory.[2]" This effort was initiated by a workshop led by the SFA that generated a number of science questions that could be addressed using the WHONDRS OM chemistry dataset. The overview article and three community contributions have been published; other contributions from the community are in review or in preparation.
- ICON/FAIR AGU Collection: The SFA organized a special collection hosted by the AGU open access journal *Earth and Space Science*. The collection, entitled "*The Power of Many: Opportunities and Challenges of Integrated, Coordinated, Open, and Networked (ICON) Science to Advance Geosciences,*[3]" comprises commentary articles representing different geoscience disciplines as represented by 19 different AGU sections. This collection was initiated in FY22 and completed in FY23.

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[1] https://jgi.doe.gov/csp-2020-microbial-genomes-across-world-rivers/

[2] https://www.frontiersin.org/research-topics/23353/crowdsourced-understanding-of-global-river-organic-matter-composition-through-the-lens-of-ecological-theory

[3] https://agupubs.onlinelibrary.wiley.com/doi/toc/10.1002/(ISSN)2333-5084.ICON

- PyOM Community Review Paper: Allison Myers-Pigg is leading the development of a community review paper on the topic of "*Shaping the future of wildfire science: Top priorities and unanswered questions on the cascading watershed impacts of fires.*" The development of the manuscript is engaging a broad spectrum of researchers using a crowdsourced approach.
- ESS University FOA: We partnered with Virginia Tech and Washington State University on a proposal to study impacts of benthic biofilms on stream metabolism, and partnered with USGS on two proposals, one focused on non-perennial streams in the YRB and another on using YRB DOM data as part of a CONUS-wide synthesis effort.
- RDPP and RENEW Programs: The SFA is actively participating in new BER programs aimed at increasing participation in BER research programs by underrepresented institutions and populations. We supported the successful RDPP proposal of Allison Veach (UTSA). We hosted her team at PNNL for training and provided specialized field equipment developed by our RCSFA and we continue to support her team in sample analysis and data interpretation.
- Engagement with Yakima River Basin Stakeholders: We have made significant progress in engagement with a variety of stakeholder institutions in the Yakima River Basin. The SFA regularly participates in meetings of the Yakima River Basin Water Enhancement Project (https://www.usbr.gov/pn/programs/yrbwep/) coordinated by the US Bureau of Reclamation, and of the Yakima River Water Quality and Habitat Coordination Group coordinated by the Benton Conservation District (https://www.bentoncd.org/copy-of-projects). In addition, we are collaborating closely with the agencies to mutually enable field efforts, such as through shared instrumentation and co-design of field efforts. We have received formal permission from the Yakama Nation Tribal Council to perform field work on tribal lands, and we frequently interact with scientists from the Yakama Nation Fisheries including participation by their staff in our field activities. We have held multiple discussions with the Yakama Nation regarding how they might use data from our field efforts and how they would like to be acknowledged in published data packages and peer-reviewed manuscripts as large portions of SFA data come from their lands. We have made contacts at Heritage University, a Native American and Hispanic-serving institution with campuses in Toppenish WA (on Yakama Nation lands) and Pasco WA (in the Tri-Cities) and have developed joint proposals and student internship possibilities. SFA staff visited the Yakama Nation Tribal School twice in FY23 and have developed relationships with students and teachers that may lead to future internships. The Yakima Valley College in collaboration with the Cowiche Canyon Conservancy invited one of our team members to present on the RCSFA's research. This event was free and open to the community which allowed us to share our science and make connections with a wider audience.
- ICON-ModEx Activity and Classroom Engagements: This activity, supported by additional year-end funds provided in FY22 and FY23, leveraged data from WHONDRS campaigns to generate ML models of riverbed respiration across the CONUS (in collaboration with ParallelWorks through an SBIR-funded project). We have engaged with the science community in monthly iterations in which ML models are used to guide sample collection, samples are crowdsourced and analyzed at PNNL, and new data are used to update ML models in a tight ModEx loop. As part of this activity we have conducted several virtual classroom engagements in which university professors have invited SFA staff to present information on the ICON-ModEx activity and sampling protocols, and then students have engaged in sampling activities.

APPENDIX C: REFERENCES CITED

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