

Understanding Spatial Patterns and Impacts of Hydrologic Exchange and Microbial Community Function from Reaction to Basin Scales

Jesus Gomez-Velez^{1*}, Kelly Wrighton², Xingyuan Chen³, James Stegen³, Emily Graham³, Tim Scheibe³ and the PNNL SBR SFA Team

¹Vanderbilt University, Nashville, TN; ²Colorado State University, Fort Collins, CO; ³Pacific Northwest National Laboratory, Richland, WA

Contact: (tim.scheibe@pnnl.gov)

Project Lead Principal Investigator (PI): Tim Scheibe

BER Program: SBR

Project: PNNL SBR SFA

Project Website: <https://sbrsfa.pnnl.gov>

The PNNL SBR SFA is employing principles of ICON/FAIR science and iterative multiscale model-data integration (multiscale ModEx) to build observational networks and numerical models that will enable predictive understanding of river corridor processes from reaction to basin scales. Hydrologic exchange flows (HEFs) and inputs of DOM (amount and molecular properties), nutrients, and contaminants are becoming widely recognized as key factors that influence microbially-mediated reactions in river corridors. However, these factors and responses vary tremendously through space and time across large river basins, making it very difficult to predict their cumulative impacts at watershed to basin scales. We are taking advantage of recent advances in theory, observational capabilities, and numerical modeling to develop interconnected observational networks across multiple large basins in the contiguous U.S. (CONUS) linked to multiscale numerical models in an iterative learning cycle. The NEXSS model has been used to predict HEFs and associated reaction potential across the CONUS, leading to new hypotheses about their distribution across river networks. This information will be combined with basin- scale functional classification of individual catchments using machine learning (ML) to guide the design of field observations and sample collection based on community-based open science approaches developed by the WHONDRS consortium. Resulting metagenomics and metabolomics data will inform reaction-scale models in PFLOTRAN using new theory, KBase workflows, and ML-based surrogate modeling being developed in collaboration with an SBIR project and the IDEAS project. Execution of these models, driven by local estimates of inputs derived from watershed model predictions and tested using laboratory experiments, will generate spatially-distributed estimates of locally-tailored reaction rates, extensible to non-sampled locations based on catchment properties (functional classification). These will, in turn, be assimilated into our river corridor modeling system (MRMT-SWAT-R) to produce updated predictions of basin-scale cumulative effects of river corridor reactions. These updated predictions will be used to refine hypotheses and observational network design, thus completing the iterative cycle of multiscale ModEx. The explicit integration of new reaction-scale understanding into watershed models in this manner offers the potential to quantify cumulative influences of HEFs and molecular properties with enhanced and robust predictive power.