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Functional Enzyme-Based Approach for Modeling Aerobic Respiration Processes in Hyporheic Zone Sediments Subject to Variable Inundation History

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This element of the PNNL SFA seeks to understand the control exerted on biogeochemical reactions by hydrologic exchange flows and translate that understanding into predictive genome-informed biogeochemical process models. Seasonal and inter-annual changes in large-scale water supply, combined with the modulating influence of highly variable releases from hydropower facilities, can give rise to large changes in river surface elevation (stage) across a spectrum of time scales. Therefore, riverbed sediments in the parafluvial zone are continually subjected to cycles of inundation and drying. SFA research has recently revealed that organic carbon speciation and transformation rates depend on time lags in aerobic respiration associated with inundation history. We have also developed a new enzyme-based biogeochemical modeling approach that accounts for microbial regulation, and successfully applied that approach to simulate denitrification processes. Proposed research will develop new and modified reaction models that will account for thermodynamic principles as well as fundamental biological mechanisms responsible for metabolic response lags. These reaction networks will be expanded from our current denitrification model to represent processes governing carbon speciation and transformations, and will involve redox pathways of nitrogen and other secondary metabolites to complete reaction paths. Based on the reasoning that biogeochemical dynamics are related to compositional status of a microbial community, we will split the community population into multiple (initially two) microbial groups characterized by different dynamic time scales: 1) oligotrophs that preferably grow at low concentration of nutrients and show long time lags and 2) copiotrophs that preferably grow at high concentration of nutrients and show brief time lags. Processes governing historical contingencies will be represented in terms of microbial response lag as a function of relative abundance of these two groups, which will vary depending on the inundation history. Reaction model development will be informed by new understanding from FTICR-MS carbon characterization, microbial genome annotation and analysis, and field-based process studies, and the resulting models will be incorporated into high-resolution reactive transport simulations of biogeochemical processes in canonical hydromorphic structures. Those simulations will enable translation of new fundamental process knowledge into predictive understanding of system behavior at larger scales.