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Reactive Transport Modeling for Watershed Carbon and Nitrogen Cycling

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Watersheds play significant roles in modulating carbon and nitrogen cycling and removal of excess nutrients. The incorporation of hydrologic complexity and molecular-level characterization such as organic carbon speciation will greatly improve a watershed hydrobiogeochemical model in capturing distinct water quality signatures across variations in land use, hydrogeology, climate, and disturbances. We have developed a modeling pipeline that connects molecular characteristics with biogeochemical models and watershed reactive transport models. The organic carbon speciation inferred from FTICR-MS measurements is used to generate new reaction networks and kinetics, which are subsequently tested in PFLOTRAN in batch and column configurations before incorporated into ATS-PFLOTRAN for coupled hydrologic and biogeochemical modeling at the watershed scale. We used this coupled model to study biogeochemical transformations of carbon and nitrogen in a few watersheds across the Yakima River Basin, located in the Pacific Northwest region of the United States. The biogeochemical hot spots and hot moments within the river corridors were found to be strongly influenced by riverbed properties and flow conditions, and hence, influenced by variations in land use, hydrogeology, climate, and disturbances. This pipeline can be extended to allow the incorporation of other omics datasets (such as metatranscripts, metaproteomics and metabolomics) when they become available. We also note that ATS-PFLOTRAN is an example of interoperable model development, where generic interfaces such as the Alquimia biogeochemistry interface library, extend the capabilities available from single codes in the software ecosystem by bringing their complementary capabilities together. We have shared our modeling pipeline with the broader community to enable similar hydrobiogeochemical studies in other watersheds and river corridors.