Linking Molecular Characterization with Continuum Reactive Transport Modeling

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Project: **IDEAS-Watersheds**

Project Website: https://ideas-watersheds.github.io/

Project Abstract:

The IDEAS-Watersheds focuses on developing flexible modeling capabilities and workflows through contributions to a community-driven software ecosystem that advance hydrobiogeochemical research in watersheds and river corridors.These contributions are in turn made available to the broader community. For example, we have developed a modeling pipeline from molecular characteristics, such as organic carbon speciation, to biogeochemical models and to continuum reactive transport models. Leveraging the DOE's KBase modeling platform, we have prototyped the two key steps of this pipeline as KBase Apps using the KBase Software Development Kit: one for translating chemical compositions from FTICR-MS into biogeochemical reaction models, and one that takes those reaction models and sets them up as 1-D reactive transport models with PFLOTRAN. After testing those new reaction networks and kinetics, which were informed by the organic carbon speciation, in PFLOTRAN in batch and column configurations, we incorporated those reaction models in ATS-PFLOTRAN for coupled hydrologic and biogeochemical modeling at the American River watershed. We used this coupled watershed model to investigate water, energy, and solute fluxes across the river-groundwater interface. The biogeochemical hot spots and hot moments within the river corridors are 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 have shared our KBase narrative examples with the broader community to enable leveraging the pipeline in hydrobiogeochemical studies on other watersheds and river corridors. Finally, we note that the

ATS-PFLOTRAN coupled watershed model 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.