Integration of Omics into a New Comprehensive Rate Law for Competitive Terminal Electron-Accepting Processes in Reactive Transport Models: Application to N, Fe, and S in Stream and Wetland Sediments

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Project Abstract: The dynamic of biogeochemical processes regulating nutrient and contaminant release in stream and wetland sediments and their role in carbon transformation cannot be predicted accurately by current reactive transport models (RTMs). These models largely rely on detectable changes in geochemical conditions to activate metabolic processes, are unable to accurately account for competition between microbial processes, and poorly constrain the effect of hydrological perturbations on biogeochemical processes. The objectives of this project are to: (i) develop new rate laws for RTMs that rely on a combination of high throughput omics (meta-genomic, -transcriptomic, -proteomic, -bolomic) and geochemical signatures to identify the underlying anaerobic microbial processes in stream and wetland sediments; (ii) describe the competition between the dominant metabolic processes involved in contaminant (U and Hg) mobilization; and (iii) more accurately quantify carbon transformation processes. A combination of meta-omic and geochemical signatures were used to identify the main anaerobic microbial processes in a Savannah River Site wetland (SRS) and Oak Ridge East Fork Poplar Creek (EFPC) sediment. Geochemical depth profiles suggested that Fe(III) reduction dominates carbon remineralization processes in SRS wetland sediments, whereas a combination of NO_3^- and Fe(III) reduction dominates EFPC sediments. Sediment slurry incubations designed to investigate the competition between anaerobic terminal electron accepting processes demonstrated that NO_3^- reduction was the fastest respiratory process and that Fe(III) reduction apparently became dominant once NO_3^- was depleted. Incubations also revealed that SO_4^{2-} reduction was inhibited by Fe(III) reduction and that this inhibition was enhanced by ferrihydrite addition. In turn, metagenomic signals were enriched in gene variants indicating that bacteria coupling anaerobic $\sum H_2S$ oxidation to NO_3^- reduction were dominant in EFPC sediments but not in SRS wetland sediments. Metagenomic data thus indicate that a cryptic sulfur cycle may be more significant than apparent by geochemical signals. The metagenomic data is currently being confirmed via complementary meta-transcriptomic and -proteomic analyses. A gene-centric kinetic model was developed that includes a set of new