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

Martial Taillefert[1*] (PI), Anthony D. Boever[1], Eryn M. Eitel[1], Thomas J. DiChristina[2] (co-PI), Hyun-Dong Shin[2], Frank Stewart[2] (co-PI), Anthony D. Bertagnolli[2], Kenneth M. Kemner[3] (Co-PI), Daniel I. Kaplan[4], Scott Brooks[5] (Co-PI), Christa Pennacchio[6], and Stephen J. Callister[7]

[1]School of Earth and Atmospheric Sciences, Georgia Institute of Technology, Atlanta, GA 30332
[2]School of Biological Sciences, Georgia Institute of Technology, Atlanta, GA 30332
[3]Biosciences Division, Argonne National Laboratory, Argonne, IL 60439
[4]Environmental Biogeochemistry & Technology, Savannah River National Laboratory, Aiken, SC 29808
[5]Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831
[6]Joint Genome Institute, Walnut Creek, CA 94598
[7]Environmental Molecular Science Laboratory, Richland, WA 99354

Contact: (mtaillef@eas.gatech.edu)
Project Lead Principal Investigator (PI): Martial Taillefert
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Project Abstract: The dynamic of biogeochemical processes in 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, do not accurately describe microbial competition, 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; and (iii) quantify carbon transformation under varying hydrological conditions. A combination of meta-omic and geochemical signatures identified the main anaerobic microbial processes in a Savannah River Site (SRS) wetland and Oak Ridge East Fork Poplar Creek (EFPC) sediment. Geochemical depth profiles suggested that Fe(III) reduction dominates biogeochemical 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 microbial processes demonstrated that NO_3^- reduction was the fastest respiratory process and that Fe(III) reduction 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. Metagenomic signals were enriched in gene variants indicating that bacteria couple anaerobic $\sum H_2S$ oxidation to NO_3^- reduction in EFPC but not SRS sediments. Metagenomic data thus indicate that a cryptic sulfur cycle may be more significant than apparent by geochemical signals in EFPC sediments. Geochemical and genomic data of SRS incubations instead point towards

outcompetition of sulfate-reducing bacteria for carbon substrate by iron-reducing bacteria. The metagenomic data is currently being confirmed via complementary meta-transcriptomic and -proteomic analyses. A gene-centric kinetic model was developed with new rate laws to account for competition between microbial communities. The model calibrated with one set of incubations was able to reproduce all SRS incubation treatments and indicated carbon substrate competition as the main control of anaerobic metabolic processes. Overall, this project demonstrates that: (i) a combination of high throughput omic and geochemical data is needed; and (ii) simple gene-centric models can be readily included in RTMs to accurately identify biogeochemical processes and microbial community competition in sediments. The role of hydrological processes on sediment biogeochemistry in gaining and losing stream SRS sediments is currently being characterized.