Title: Developing a probabilistic framework to capture redox heterogeneity and greenhouse gas predictions in Terrestrial-Aquatic Interfaces

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Project Abstract: Terrestrial-Aquatic Interfaces (TAIs) represent dynamic transition zones between land and water, where steep physical, chemical, and biological gradients converge for accelerated biogeochemical transformations and greenhouse gas (GHG) emissions. Hydrological dynamics strongly affect redox conditions that drive the transformations of redox-sensitive elements such as nitrogen (N), dissolved organic matter (DOM), iron (Fe), manganese (Mn), and sulfur (S). These transformations impact soil organic matter (SOM) decomposition and GHG emissions. Currently, these complex interconnected processes remain underrepresented in ecosystem and Earth system models (ESMs) because we lack modeling tools that can directly constrain and parameterize heterogeneity in redox processes that vary at highly condensed spatial and temporal scales. To address this gap, we are building a dynamic modeling framework that captures the heterogeneity at microsite-scales, which drives hot spots and hot moments of GHG emissions at ecosystem scales across TAIs. We leverage probability density functions (PDFs) to capture numerically the spatiotemporal heterogeneity of soil microsites needed to predict non-normal distributions of microbial activity. We hypothesize that modeling of plot-scale and ecosystem-scale dynamics of GHGs can be improved by integrating and upscaling microbial metabolic activities at the microsite-scale. Our new modeling framework (Redox-DAMM) merges the capabilities of microsite PDFs of the DAMM-GHG model (Dual Arrhenius and Michaelis Menten-GreenHouse Gas, Sihi et al., 2020, Global Change Biology, DOI: 10.1111/gcb.14855) with a redox reaction network model (Zheng et al., 2019, Biogeosciences, DOI: 10.5194/bg-16-663-2019). The Redox-DAMM framework contains three key components: (1) Microsite PDFs, (2) PDF-constrained redox reaction networks, and (3) Redox reaction networks within the soil pore-network that inform diffusion-limitation of substrates related to the production and consumption of GHGs. Soil heterogeneity represents an important, yet unresolved, component in biogeochemical models. We will demonstrate that dynamic representations of redox heterogeneity improve model performance of GHG emissions in TAIs. Microsite PDF function-based computational tools represent a great advance in generating transferrable modeling capability from fine-scale processes to ecosystem-scale functions, directly supporting BER priorities of understanding multi-scale Earth system dynamics and processes.