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Exploring the controls of soil biogeochemistry in a restored coastal wetland using object-oriented computer simulations of uptake kinetics and thermodynamic optimization in batch reactors

Many hypotheses have been proposed to predict patterns of biogeochemical redox reactions based on the availability of electron donors and acceptors and the thermodynamic theory of chemistry. Our objective was to develop a computer model that would allow us to test various alternatives of these hypotheses against data gathered from soil slurry batch reactors, experimental soil perfusion cores, and in situ soil profile observations from the restored Timberlake Wetland in coastal North Carolina, USA. Software requirements to meet this objective included the ability to rapidly develop and compare different hypothetical formulations of kinetic and thermodynamic theory, and the ability to easily change the list of potential biogeochemical reactions used in the optimization scheme. For future work, we also required an object pattern that could easily be coupled with an existing soil hydrologic model. These requirements were met using our recently developed Network Exchange Objects (NEO), an object-oriented distributed modeling framework that facilitates simulations of multiple interacting currencies moving through network-based systems.

An initial implementation of the object pattern was developed in NEO based on maximizing growth of the microbial community from available dissolved organic carbon. We then used this implementation to build a modeling system for comparing results across multiple simulated batch reactors with varied initial solute concentrations, varied biogeochemical parameters, or varied optimization schemes. Among heterotrophic aerobic and anaerobic reactions, we have found that this model reasonably predicts the use of terminal electron acceptors in simulated batch reactors, wherein higher energy yielding reactions occur before the lower energy yielding reactions. However, among the aerobic reactions, we have also found this model predicts dominance of chemoautotrophs (e.g., nitrifiers) when their electron donor (e.g., ammonium) is abundant, despite the fact that aerobic respiration produces a higher energy yield from the available dissolved oxygen. This suggests that incorporation of an alternative hypothesis, such as a maximum efficiency model, may be necessary to explain an observation of substantial aerobic respiration occurring in the presence of high ammonium and oxygen concentrations. We will test this model against results from batch reactor experiments that have treated soil slurries with a full factorial combination of various levels of reactive solutes found in freshwater (e.g., nitrate) and seawater (e.g., sulfate). Initial comparisons suggest that the model may need to account for the biogeochemical reactivity of iron and the physical influence of salt to properly describe variability in the biogeochemistry of Timberlake soils. Comparisons of these evolving models with field-derived data from soils will ultimately reveal how thermodynamic theory may be used to explain the evolution of nutrient retention and greenhouse gas emission in the Timberlake Wetland, where nutrient behavior is changing after restoration from agricultural land use and where inputs of brackish water are expected to increase due to sea level rise.