A field guide to experimenting with biogeochemical models

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A general goal of biogeochemical research is to understand the complex interactions that occur between flowing water, reacting nutrients and hungry organisms. Such understanding is often measured by our ability to "predict" certain outcomes in response to changing boundary conditions, or more often, to rigorously attribute outcomes to processes. Both usually require the use of a numerical modeling framework. In fact, some funding agencies now explicitly require projects to use or contribute meaningfully to modeling frameworks to drive continual evolution. How should we navigate the ever changing landscape of models?

Biogeochemical models are immense, but incomplete, libraries of knowledge. Our task is not only to train these models to reflect our understanding, but to use them to test ours. Numerical models require a reaction network to operate. Well-controlled experimental studies are an ideal way to build these reaction networks. Although most experimentalists may not need a numerical model to interpret their results, most models need the experiments to learn. Examples include surface complexation modeling of sorption studies to identify new surface species, and reactive transport modeling combined with flow imaging of column studies that reveal the complexity of microbial growth. Ultimately, even in simple experiments new processes are often identified by enforcing a rigorous mass balance and testing existing knowledge structures using models.

Bringing models from the laboraory to the field is where we stand to learn the most. However, both the models and research teams may benefit from adopting a more radical approach to field investigations, including the use of natural environmental gradients combined with large-scale manipulations to provide more experimental controls and ulimately more training opportunities for models. Such experimental designs are need to move beyond the “site-specific” model that emerges when we train models with limited experimental and field data. Examples can be drawn from decades of ecological manipulations that have greatly improved our ability to model the response of ecosystems to climate change, and hopefully our knowledge of the underlying processes.