MEETINGS

Expanding the Role of Reactive Transport Modeling in Biogeochemical Sciences

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Earth systems are complex due to the intimate coupling of physical, chemical, and biological processes in the subsurface. Field observation and data analysis have provided significant insights into the coupling of these processes. However, mechanistic understanding often requires advanced modeling tools to quantify the role of individual processes while maintaining the process coupling that determines the overall system behavior. As a result, reactive transport modeling (RTM) has been used extensively to interrogate complex subsurface processes relevant to energy and the environment. Existing work has shown the significant research and educational advantages of RTM in elucidating mechanisms, integrating large data sets, testing hypotheses, and guiding the stewardship and management of water and energy resources.

Despite 3 decades of successful application of RTM, widespread adoption of theory and methods into teaching and research programs has proceeded slowly. In this context, a National Science Foundation–supported workshop was held with the goal of expanding the use of RTM within the biogeosciences. The workshop considered three questions: (1) What are key outstanding hypotheses in biogeochemical sciences that could be addressed with current RTM capabilities? (2) What additional RTM capabilities would expand the scope of scientific hypotheses that could be addressed? (3) What educational tools are critically needed but not widely available, and how should these be developed?

Twenty-five researchers, including three graduate students and two postdocs, gathered for the workshop. Among the participants were scientists with broad disciplinary strengths, including numerical methods for large-scale data collection and analysis. Five speakers highlighted new advances and technical challenges in RTM. The remaining participants each presented 5-minute perspectives talks highlighting a key scientific question uniquely addressed through the application of RTM approaches. Finally, a survey was developed to capture broader perspectives regarding RTM use and education; it was distributed to a broad cross section of the biogeochemical science community.

The discussions focused on identifying the research, educational, and infrastructure needs to support continued growth of RTM. Four research directions were highlighted. The first is to expand RTM to longer temporal and larger spatial scales to allow for more rigorous evaluation of the formation and evolution of the critical zone over geological time scales (~10^4 to ~10^6 years). Model development in larger spatial scales is needed to interface with other Earth system models, including land-surface models, surface water–groundwater models, and atmosphere-ocean global climate models.

The second identified direction includes model developments for root zone processes that capture the coupling among roots, microbes, organic carbon, water, and minerals. The third research area includes the development of capabilities for incorporating the rich genomics and proteomics data emerging from omics technologies in microbiology. Ideally, fundamental concepts and knowledge gained from massive omics data sets can be used to interrogate the evolution and function of microbial communities.

The fourth direction includes the RTM expansion for rigorous treatment of isotope fractionation to trace key biogeochemical processes. Discussion of RTM education focused on linking existing resources and creating a larger scientific community that employs RTM as a research tool.

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