Expanding the Role of Reactive Transport Modeling (RTM) within the Biogeochemical Sciences

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The formation, operation, and evolution of Earth systems are complex due to the coupling of physical, chemical, and biological processes in the subsurface. Data collection and analysis coupled with field observation have provided significant insights into the factors that determine the evolution of the critical zone. Mechanistic understanding and prediction of the intimately coupled processes, however, often requires advanced modeling tools that can integrate large and diverse data sets to quantify the effects of individual processes, while at the same time provide a window into the coupled processes that may control the overall system behavior. Reactive Transport Modeling (RTM) has been used for approximately three decades to understand complex subsurface processes in many applications, including weathering and soil formation, remediation, natural attenuation, and geological carbon sequestration. RTM is now also becoming essential for the understanding of key societal issues such as “fracking”.

We organized an NSF workshop on April 13-15 in Embassy Suites Hilton in Alexandra. The goals were to (1) identify the frontiers of reactive transport in the biogeochemical sciences, and (2) determine what educational and infrastructure development is required to achieve these goals. We aimed to identify key interfaces between reactive transport modeling approaches and biogeochemical data collection and analysis. Some of the key questions included 1) What are key outstanding hypotheses that could be addressed with current capabilities? 2) What are additional modeling capabilities that would expand the scope of scientific hypotheses that can be addressed? 3) What educational tools are critically needed but are not available, and how should these be developed?

There have been a lot of interesting discussions during the RTM workshop along these lines. Currently RTM has typically been used in subsurface systems within a range of scales typically from the pore scale (10-5 meters) to field scales (10s of meters). However, the community is really pushing forward to see the coupling between subsurface RT processes to various other processes, including surface hydrology, plants, land-surface interactions, ecosystems, carbon cycling at a wider range of scales from as small as a cell to as large as the global scale. The discussions on education focused on what can be done to teach more RTM courses and help maintain the momentum for biogeochemists to include RTM in their research toolboxes.