

Reactive transport modeling for evaluation and optimization of architected materials

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Reactive transport modeling offers a powerful tool for evaluating and optimizing architected materials. Architected materials are essentially synthetic rock analogues that can show controlled and/or understandable geochemical behavior, in many cases without all of the complexity of natural geological materials. In other words, the materials can be designed so that complexity is controlled. There are several possible roles for reactive transport modeling (RTM), which of course can be thought of as model systems applied to virtual synthetic mineralogical and geochemical systems. One important role for RTM is pre-modeling for the purpose of material and experimental design such that the cost of fabrication, characterization, and experimentation are minimized. A second role for RTM is to carry out sensitivity analyses so as to choose material properties and experimental conditions such that the “signal” is maximized—this reduces the likelihood that a potentially expensive experiment is performed that yields very little information because of a poor choice of conditions. A third role is in the interpretation of more complex architected materials, since even though they are synthetic, their behavior may still be difficult to unravel.

As an example, we consider two model systems: 1) one involving ion transport subject to electrostatic effects in clay and clay-rich rock, and 2) carbonate mineral trapping in synthetic subsurface materials due to the injection of CO₂. We present some examples in which modeling can be used to optimize the design of the material and associated experiments and characterization.