

Microcontinuum modeling of CO₂-water-rock interaction

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To know the total amount of carbon that can be trapped in mineral form and the effects of CO₂ injection on the properties of subsurface formations requires that we are able to predict mineral reaction rates in natural porous media. However, most kinetic studies of mineral dissolution and precipitation have been carried out in well-stirred reactors in the laboratory, where both transport effects (e.g., partial diffusion control) and “porous media” effects (e.g., restricted and/or inaccessible pores) are absent. Here we introduce a microcontinuum modeling approach that builds on high resolution microscopic imaging that can be to investigate the extent to which the 3-5 orders of magnitude lab-field discrepancy is due to porous media effects. The approach is applied to the study carbonate mineral trapping rates in the lower Tuscaloosa Formation at the Cranfield pilot injection site in Mississippi. Bulk reaction rates in the heterogeneous sediment are estimated by carrying out 2-D diffusion-reaction simulations using volume-averaged porosity and mineral distributions determined based on 2-D Back Scattered Electron-Scanning Electron Microscopy (BSE-SEM mapping.. The 2-D BSE-SEM data was augmented by 35 nm resolution FIB-SEM characterization of nano-porous chlorite zones, which was then used as the basis for numerical simulations to estimate effective diffusion coefficients for the material. The sparse distribution, limited connectivity, and low diffusivity of chlorite in the sediment all contribute to the low bulk reactivity of the sandstone.

A second effort involves the interpretation of detailed characterization data from the Nagaoka Formation in Japan, the site of a pilot CO₂ injection field experiment. In this study, a range of reactive surface area estimates were developed and evaluated for their ability to predict dissolution rates in well-stirred and intact core reactor experiments. Reactive transport modeling was used to determine which of a number of reactive surface area models provide the best match with the effluent chemistry. The closest match with the well-stirred experiment were obtained by using specific surface area estimates from a newly developed image-based approach, while the porosity-accessible reactive surface area (10 to 20X lower) provides the best match to the intact core data.