Coupling Between Flow and Precipitation In Heterogeneous Subsurface Environments and Effects on Contaminant Fate and Transport (Project no. 99272)

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Abstract

This project is aimed at understanding how contaminant transport in heterogeneous porous media is impacted by precipitation and dissolution events through chemical interactions with precipitates and as a consequence of coupling between precipitation and flow. We hypothesize that precipitation/coprecipitation, encapsulation, isostatic from flow and alteration of reactive surfaces will contribute to altering contaminant mobility during precipitation events, and that predicting the release of contaminants during precipitation events requires an understanding of how precipitates are distributed and how contaminants are released from the different compartments over time. Using calcium carbonate as a model system, physical experiments and modeling at the pore-scale and continuum-scale will be used to improve the conceptual approach to predicting the impact of dissolution events on solute migration. Column and 2-dimensional intermediate-scale experiments with constructed physical and chemical heterogeneities will be used to investigate the movement of fluids and reactive solutes during different types of mixing events that lead to calcium carbonate saturation and precipitation. Smoothed particle hydrodynamic modeling will be used to simulate pore-scale mixing and precipitation in heterogeneous porous media and estimate continuum-scale parameters. Continuum-scale modeling will be used to test conceptual models and associated effective parameters that simulate the macroscopic behavior of the experimental domains.

Models for Proposed Experiments

Our goal is to understand how precipitation and dissolution in heterogeneous porous media can impact the short- and long-term transport behavior of reactive metal contaminants. The impact is expected to occur through structural changes in permeability that affect the rate of fluid and solute transport between high and low permeability zones, and through direct interactions between the precipitate and contaminant. Macroscopic, continuum-based modeling of column and intermediate-scale 2-D experiments will be used to characterize, via effective parameters, the averaged transport behavior of fluids and a reactive solute, strontium. Pore-scale modeling and bulk-scale 2-D experiments will be used to test hypotheses concerning relationships between reaction kinetics, the distribution of precipitates, and solute transport.

Preliminary Work

- Precipitation at mixing fronts
- Model applications
- Analytical methods including x-ray tomography, complex resistivity.

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Figure 1. 2-D cell at INL. Modular inlet and outlet port configurations along all sides allow great flexibility in experimental design.

Figure 2. Demonstration of parallel flow, using inert dyes. Mixing occurs at the interface, and the mixing zone widens due to dispersion.

Figure 3. Examples of precipitate morphologies observed at different locations in mixing zone between parallel flows of CaCl₂ and Na₂CO₃.

Figure 4. Demonstration of flow impedance due to calcite precipitation. Inert dye injected perpendicular to original parallel flows of reactants (introduced from the bottom). Dye impeded most near start of original mixing zone; farther into the zone, permeability was less affected.

Figure 5. Macroscopic simulation of solute mixing along interface of parallel flows of reactants. Figures on right show calcite saturation conditions for the condition of parallel flows of reactants.

Figure 6. SPH simulation of precipitate formation at interface between parallel flows of reactants, coming from bottom.

Figure 7. SPH simulation of precipitation due to infiltration (from the top) of a supersaturated solution into a high permeability channel.