Understanding and Controlling Precipitation Reaction Fronts in Subsurface Environments: The Idaho National Laboratory SBR Scientific Focus Area

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Although subsurface environments are repositories for many of the most critical energy, water and mineral resources that sustain the earth's ecosystems and human populations, it remains a persistent challenge to exploit subsurface resources without unintended and undesirable consequences. Geochemical processes in subsurface environments dictate the quality of subsurface resources and the response of the subsurface to contaminants, resource extraction practices or changing ecosphere conditions. Consequently, engineered geo- and biogeochemical processes are now instrumental in efforts to stimulate subsurface reactions to enhance resource recovery or prevent and mitigate damage caused by engineered or accidental interventions in the subsurface.

Possible chemical responses of the subsurface to inputs can be predicted from knowledge based on controlled laboratory studies. However, deliberate stimulation of chemical and biochemical processes in the subsurface usually involves the injection and dispersal of reactants or catalysts where mixing of fluids and reactants become important. The porous and fractured nature of the subsurface creates transient reactant mixing patterns and thermodynamic gradients. The spatial-temporal distribution of reactions is complex particularly when the transport properties of the subsurface are changed through formation of precipitates or biomass.

The theme for the Idaho National Laboratory (INL) Scientific Focus Area (SFA) is "Understanding and Controlling Precipitation Reaction Fronts in Subsurface Environments." We are investigating how different modes of reactant mixing in porous media affects the spatial and temporal distribution of reaction products with a special focus on reactions that include precipitation of mineral phases. The scientific challenge is to understand the relationship between pore-scale processes and their manifestation at large scales. The engineering challenge is to understand how reactions can be propagated in complex heterogeneous media to produce the desired outcomes with respect to targeted outcomes. The INL SFA research program addresses a number of challenging and interrelated topics: The transport and mixing of reactants at multiple scales in porous and fractured media; Relationships between fundamental reaction rates and macroscopically observed and modeled volume averaged reaction rates; The complex behavior of systems where physical processes affecting transport and reactant mixing are tightly coupled to chemical and biogeochemical processes, and; Novel methods that can be used to noninvasively monitor mixing-reaction fronts in subsurface environments.

In the final year of the INL SFA, we are focusing on: 1) how mineral ($CaCO_3$) precipitates are formed within the mixing interface between solutions flowing in parallel, 2) how mineral precipitates are formed in mixing zones controlled primarily by diffusion, 3) $CaCO_3$ precipitation reaction fronts generated when a reactant (carbonate ion) is formed in situ by enzymatic hydrolysis of urea, and 4) whether complex resistivity can be used to monitor the position and composition of reaction fronts. Each research area is supported through a modeling platform that is well suited for the simulation of tightly coupled processes because the chemical reactions induce changes in the transport properties of the porous medium. The principles being addressed in the INL SFA will contribute to better predictions for biogeochemical processes where mixing and strong chemical gradients occur in nature or in engineered systems.