

## **Mineral Precipitation Fronts in Porous Media: Modeling using A Fully-coupled Fully-implicit Simulator and Monitoring using Spectral Induced Polarization (SIP)**

Chi Zhang<sup>1,2</sup>(chi.zhang@inl.gov), Luanjing Guo<sup>2</sup>, George Redden<sup>2</sup>, Hai Huang<sup>2</sup>, Don Fox<sup>2</sup>,  
Yoshiko Fujita<sup>2</sup>, Lee Slater<sup>1</sup>, Timothy Johnson<sup>3</sup>

1. Dept. of Earth and Environmental Sciences, Rutgers University-Newark, Newark, NJ, 07102

2. Idaho National Laboratory, Idaho Falls, ID 83415

3. Pacific Northwest National Laboratory, Richland, WA 99352

Groundwater contamination by toxic and/or radioactive metals is often untreatable when extraction methods are ineffective or the contaminated environment is inaccessible. This situation has driven the need to develop methods that can immobilize inorganic contaminants *in situ*. Successful development and application of *in situ* remediation requires the ability to simulate the various physical, chemical and biological processes that will govern contaminant state and mobility. These processes are often closely coupled, particularly where precipitation reactions modify physical properties of the media governing transport. It is also necessary to monitor the associated changes in physicochemical properties that are caused by the engineered introduction of amendments in the subsurface.

Experiments involving calcium carbonate precipitation induced by enzyme-driven urea hydrolysis have been carried out in granular silica gel columns where urease enzyme was adsorbed on silica within a defined segment of the column. Experimental measurements were taken for the spatio-temporal distribution of urea, ammonium ( $\text{NH}_4^+$ ), pH and calcium carbonate precipitation. They have been used to investigate the dynamics of mineral precipitation reaction fronts in porous media, and to develop and test approaches for simulating and monitoring the transient features of reaction fronts. A fully-coupled, fully-implicit reactive transport simulator has been applied to investigate the nonlinear coupling effects between the processes of flow, transport and reaction, as well as the interaction between mineral precipitation and medium properties. Simulation results were compared to the lab measurements. Good agreement between most of the experimental and simulated results suggests that the model successfully accounts for the most important processes in the system and can be used to make reasonable predictions of outcomes for scenario testing.

We have been evaluating spectral induced polarization (SIP) for delineating spatio-temporal variations in reaction front chemistry and the properties of the grain surface-fluid interfaces. Complex resistivity was tested as a method for monitoring the progress of the precipitation reaction fronts in the column experiments. Correlations were found between the increased real ( $\sigma'$ ) and imaginary ( $\sigma''$ ) parts of complex conductivity and the increase in hydroxide ion concentrations during urea hydrolysis. Additionally, decreased complex conductivity was observed as calcite precipitation proceeded. The spatiotemporal variations in complex conductivity suggest polarization mechanisms were associated with changes in the interfacial properties of a solid-fluid surface. Based on our observations as well as support from additional experimental work we propose a conceptual model describing hydroxide ion adsorption behavior in silica gel and its control on interfacial polarizability. Our results demonstrate the application of both modeling and geophysical sensing to facilitate an improved understanding of the dynamics of mineral precipitation reaction fronts in the subsurface.