# Reactive Facies: An Approach for Parameterizing Plume-scale Reactive Transport Models Using Multi-type Multi-scale Datasets

*LBNL SFA (Laboratory Research Manager: Susan Hubbard)*

H.M. Wainwright, D.S. Sassen, S.A. Bea, J. Chen and S.S. Hubbard (PI) – *LBNL*

Predicting subsurface contaminant plume evolution and natural attenuation is challenging due to the difficulty to tractably characterize heterogeneity of flow and transport properties. This study explores a concept of reactive facies, which is based on the hypothesis that we can identify geological units that have unique distributions of reactive transport properties. Because geophysical attributes are often sensitive to delineate such geological units, this concept allows us to take advantage of both laboratory studies and field geophysical/lithological datasets to characterize the spatial distribution of reactive transport parameters. This concept is expected to be especially powerful for characterizing coupled physiochemical parameters over large spatial regions, where it is typically challenging to obtain information about reactive transport parameters with sufficient resolution for numerical reactive transport simulations.

The first part of this study focuses on testing the reactive facies concept at the Department of Energy uranium contaminated Savannah River Site F-Area, where we have analyzed the relationships between laboratory and field (including crosshole radar and seismic, and surface seismic) datasets. First, data mining and iteration with laboratory analysis identified two reactive facies that have unique distributions of mineralogy, texture, hydraulic conductivity and geophysical attributes. We then used these correlations within a Bayesian framework to integrate the crosshole geophysical datasets with the sparse core-based measurements. This yielded high-resolution estimates of reactive facies and their associated reactive transport properties in the scale of crosshole geophysical measurements. To illustrate the value of reactive facies, we simulated migration of an acidic-U plume through this domain. The modeling results suggested that each identified reactive facies exerts a unique control on plume evolution, highlighting the usefulness of the reactive facies concept for spatially distributing reactive transport properties.

The second part of this study presents a stochastic-estimation framework for assimilating multi-source and multi-scale datasets and characterizing a plume-scale subsurface domain. The challenges are to (1) honor the large-scale variability without smoothing out the detailed structure of facies, and (2) assimilate multi-source, multi-scale datasets in a systematic way. To tackle these challenges, we developed a multi-scale Bayesian estimation method to combine disparate wellbore and geophysical datasets having varied resolution and spatial coverage. The model represents multi-scale heterogeneity by a tree-based multi-scale indicator field, and uses Markov-chain Monte-Carlo sampling methods to estimate the marginal posterior distribution of the reactive facies fields. We tested the developed method in synthetic studies and applied to the real field datasets at the F-Area, including wellbore lithology, cone penetration testing, crosshole and surface seismic data. The results showed that the point-scale and crosshole data provide the detailed structure of reactive facies in their vicinity, while the surface seismic data identify the large-scale trend and map facies with increased certainty over a large domain. We found that our methodology effectively integrates different types of data, providing an approach for distributing critical information over plume scales needed for simulating plume migration and remediation. Applying the reactive facies concept to other sites/problems would be needed to test the general utility of this approach as a new paradigm for characterizing reactive transport properties over field-relevant regions.