GEOCHEMICAL AND PHYSICAL AQUIFER PROPERTY HETEROGENEITY: A MULTI-SCALE SEDIMENTOLOGIC APPROACH TO REACTIVE SOLUTE TRANSPORT

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We hypothesize that geochemical and physical hydrologic properties that control reactive solute transport in sedimentary aquifers are correlated to lithofacies. Sedimentary lithofacies reflect the winnowing and sorting processes (erosion, transport and deposition) that create them. We approach the problem from a sequence stratigraphic perspective that provides a multi-scale framework for predicting the spatial distributions of lithofacies within a basin-scale context. If the hypothesis is correct, then quantitative information about the spatial structure of hydrophysical and hydrochemical aquifer properties, as well as relations between them, can be ascertained from knowledge of the process-based sedimentology of the system gained through modeling lithofacies distributions, combined with knowledge of the underlying variability of properties within each lithofacies.

The proposed project seeks to test the hypothesis for one site, a portion of the saturated zone at the Hanford Site (Ringold Formation), and for a model solute, carbon tetrachloride (CT). The representative geochemical and physical aquifer properties selected for quantification in the proposed project are the properties that control CT transport: hydraulic conductivity (K) and reactivity (indicated by the sorption distribution coefficient, K_d,and the anaerobic transformation rate constant, k_n). We will combine observations at outcrop analog with measurements from archived and fresh core samples from the Ringold Formation to place local-scale lithofacies successions, and their distinct hydrologic property distributions, into the basinal context, thus allowing us to estimate the spatial distributions of properties that control reactive solute transport in the subsurface. The objectives of the proposed project are to:

- Determine the significance of lithofacies in explaining the variance of K and reactivity to CT, indicated by K_d, for the Ringold Formation through intensive sampling, analysis, and rigorous statistical testing. We will also measure k_n and conduct detailed characterization of selected samples representative of saturated Ringold Formation units to characterize differences in transformation rate and the controlling geochemical properties;
- Develop a sequence stratigraphic framework for the sedimentary basin, and measure lithofacies geometries and spatial distributions, and use this to model the distribution of lithofacies at the Hanford Site through application of transition probability geostatistics at multiple scales;
- Combine the simulated lithofacies spatial distributions and the observed K, K_d and k_n for each lithofacies to create models of the spatial distributions of reactive transport properties for a portion of the CT contaminated site; and
- Use the improved site model in preliminary numerical solute transport simulations to demonstrate the effects of physical and chemical property heterogeneity on CT fate and transport in the Ringold Formation.

The research is relevant to DOE needs for methods to improve prediction and reduce uncertainty in subsurface flow and transport simulations used to evaluate long term risk, and to evaluate remediation alternatives where sedimentary aquifers are contaminated. This project embodies developing and testing methods to combine quantitative sedimentology and geochemical measurements to produce improved multi-scale hydrogeophysical and geochemical models of the subsurface environment. As such, once developed, we anticipate that the methodology will be broadly adaptable to other field sites in sedimentary aquifers. The project also carries a number of specific benefits applicable to the Hanford Site to the CT plume and to other contaminants that reside within the unconfined aquifer.

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