Objective

- Perform the first-to-date coupled pore- and continuum-scale hybrid multiscale simulation of an intermediate-scale reactive transport experiment. Demonstrate the feasibility and improved accuracy of the approach.

Approach/Results

- Pore-scale simulation of a bimolecular homogeneous reaction at the interface of two mixing fluids, in the region where continuum approximations are invalid.
- Couple to continuum-scale simulation of flow and transport over a much larger domain using a hierarchical multiscale method (Tartakovsky and Scheibe, 2011).
- Utilize the SWIFT parallel workflow environment to manage the large number of individual pore- and continuum-scale simulations and data exchange, and apply to perform an integrated complex simulation in reasonable time.

Significance and Impact

- Standard continuum models tend to overestimate the rate of reaction in a diffusion-limited mixing system. Pore-scale models can capture these processes with higher fidelity but are computationally expensive.
- The combination of continuum- and pore-scale models in a hybrid simulation provides improved accuracy while maintaining computational feasibility.