Hybrid Multiscale Simulation of a Mixing-Controlled Reaction

Objective

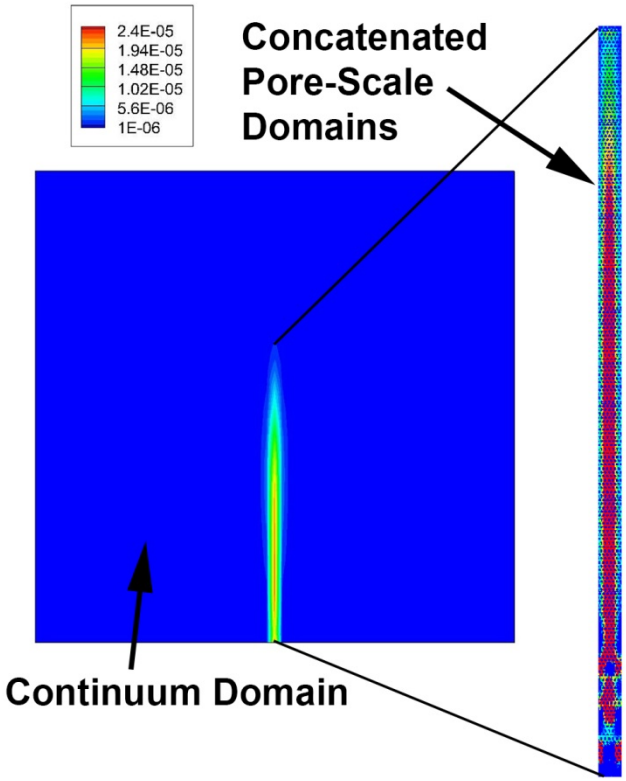
- Perform the first-to-date coupled pore- and continuum-scale hybrid multiscale simulation of an intermediate-scale reactive transport experiment. Demonstrate the feasibility and improved accuracy of the approach.

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.



Concentration contours of the simulated reaction product in the mixing interface in (left) the continuum domain and (right) the underlying pore-scale subdomains concatenated to form a single image.

Scheibe T. D., Schuchardt K., Agarwal K., Chase J., Yang X., Palmer B. J., Tartakovsky A. M., Elsethagen T. and Redden G. (2015) Hybrid multiscale simulation of a mixing-controlled reaction. *Advances in Water Resources*, **83**: 228-239, doi:10.1016/j.advwatres.2015.06.006.