Contribution ID: **619** Type: **Oral Presentation**

A Dynamic Hybrid Multiscale Model for Simulating Flow and Mixing-Controlled Reactions in Porous Media

Thursday, 3 June 2021 11:30 (15 minutes)

Mixing-controlled reactions govern various systems, and play a central role in many industrial applications (e.g., CO2 sequestration and microbially-induced calcite precipitation). However, at-scale models are limited in simulating such processes with high fidelity and computational efficiency, especially in describing those reactively "hot spots"that often occur at fundamental scales but having significant effects on larger-scale system behaviors. In this study, we present a domain-decompositon based hybrid multiscale model combined with adaptive criteria that can dynamically determine pore-scale subdomains where/when needed and simulate pore-scale and Darcy-scale processes concurrently, namely the dynamic hybrid multiscale model (dHMM). Pore- and Darcy-scale multiple-relaxation-time lattice Boltzmann models (MRT-LBMs) are loosely-coupled in an iterative way via proper boundary conditions through a multiscale universal interface. To facilitate pore-scale subdomains, a dynamic threshold calculated based on real-time concentration distribution is utilized. Simulated results are first validated by comparing with analytical solutions. The dHMM is then applied to simulate mixing-controlled bimolecular reactions in both homogeneous and heterogeneous porous media. Results are cross-compared with data computed from our previously-developed HMM and at-scale models. We demonstrate that the dHMM serves as a powerful tool for numerical upscaling and studying the effects of small-scale processes to large-scale systems.

Time Block Preference

Time Block C (18:00-21:00 CET)

References

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