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A dynamic hybrid multiscale model for simulating mixing-controlled reaction in porous media

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Pore-scale simulation that takes micro-scale architecture and mechanisms into consideration is feasible to interpret fundamental processes emerged from macro-scale systems that cannot be easily-captured by continuum-scale models. However, extreme computational costs limits the applications of pore-scale models. To bridge the gap between continuum-scale models and pore-scale models with lower cost and higher resolution, hybrid multiscale models (HMMs) are known for their flexibility of enabling micro-scale models of interest in a larger system. Nevertheless, most of the previous HMMs have only been applied to simple porous samples with fixed micro-scale domain defined a priori. In the present study, we extend our pre-developed loose-coupling HMM to incorporate adaptive criteria that dynamically determine pore-scale regions where/when needed. Both pore- and Darcy-scale multiple-relaxation-time lattice Boltzmann models (MRT-LBMs) are coupled to simulate mixing-controlled bimolecular reaction in porous media. To facilitate pore-scale domains, a dynamic decision threshold calculated based on real-time concertation distribution and the reaction rate is utilized. Simulated results are first validated by comparing with single-scale simulations in 2D synthetic porous media then further applied to study more complicated transport processes in 3D heterogeneous soil samples.