HYBRID MODELS OF REACTIVE TRANSPORT IN POROUS MEDIA

Ilenia Battiato, Clemson University, 0049015153696046, ibattiat@gmail.com

1. Ilenia Battiato, Department of Mechanical Engineering, Clemson University

Darcy-scale models of flow and transport in porous media often fail to describe experimentally observed phenomena, while their pore-scale counterparts are accurate but can be computationally prohibitive. Most numerical multi-scale models, which seek to combine these two descriptions, require empirical closures and/or assumptions on the behavior of pore-scale quantities at the continuum (Darcy) scale. We present a general formulation of an iterative hybrid numerical method that links these two scales without resorting to such approximations. The algorithm treats the fluxes exchanged at the internal boundaries between the pore- and continuum-scale domains as unknown, and allows for iteratively determined boundary conditions to be applied at the pore-scale in order to guarantee their continuity. While the algorithm proposed is general, we use it to model Taylor dispersion in a fracture with chemically reactive walls. Results show significant improvement upon standard continuum-scale formulations.