Hybrid multiscale modeling to couple pore and continuum scale processes of transport, reaction and biofilm growth along a transverse mixing zone

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Biological processes in porous media play an important role in a variety of geological and engineering applications. Native micro-organisms are normally attached to solid surfaces, and cellular metabolism often does not occur until aqueous electron donors and acceptors are brought in contact with microbes. This mixing is due to advection, diffusion and dispersion processes. As biofilms grow, pore clogging may occur, thereby altering pore-scale flow paths which in turn affects the mixing and reaction. These interactions are challenging to quantify using conventional continuum-scale models which average solute concentrations and biomass over a representative elementary volume (REV). Pore-scale models can accurately resolve coupled reaction, biofilm growth and transport processes, but modeling at this scale is not feasible for practical applications. We present a multiscale model of biofilm growth in which non-overlapping regions at pore and continuum spatial scales are coupled by a suitable method that ensures continuity of flux across the interface. Thus, regions of high reactivity where flow alteration occurs are resolved at the pore scale for accuracy while regions of low reactivity are resolved at the continuum scale for efficiency. This approach thus avoids the need for empirical upscaling relations in regions with strong feedbacks between reaction and porosity change.

We present results for simplified two-dimensional scenarios with transverse mixing of electron donors and acceptors. Many field, laboratory, and modeling studies in the literature have demonstrated that transverse mixing of nutrients along the fringes of a contaminant plume control the overall degradation rate for natural or engineered in situ bioremediation. In this case, there is a zone with high reaction rate near the contaminant source, but the reaction rate decreases and eventually becomes mixing-limited at some distance downgradient. We use pore-scale modeling in the source region and transition to continuum scale in the mixing-limited zone. We examine the impact of Peclet and Damkohler Number and discuss some challenges for modeling biomass growth and spreading near the pore to continuum scale transition.