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HYBRID MODELS FOR REACTIVE TRANSPORT IN POROUS MEDIA

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Summary. (Bio-)Chemical reactive transport processes in porous media are of ubiquitous nature in environmental systems. These processes can be described by employing either pore-scale or Darcy-scale (macroscopic) models. Pore-scale simulations have a solid physical foundation, but require the knowledge of pore geometry that is seldom available and are impractical as a predictive tool at scales that are orders of magnitude larger than the pore scale.

On the other hand, macroscopic models overcome these limitations at the cost of relying on phenomenological descriptions and/or closure assumptions. While useful in a variety of applications, such models are known to fail to capture a number of experimentally observed transport features, including, among the others, long tails breakthrough curves and extent of reactions in mixing controlled chemical transformations.

The localized nature of many physical processes (e.g. reaction fronts) calls for hybrid simulations which resolve a small reactive region with a pore-scale model that is coupled to its continuum counterpart in the rest of a computational domain.

We present a Finite Volumes numerical scheme that couples a two-dimensional pore-scale capillary tube model with its one-dimensional upscaled counterpart represented by the classical Taylor-Aris dispersion equation, generalized to incorporate heterogeneous reaction.

Pore-scale is resolved in a small portion of the domain and the coupling is performed through a flux/source matching between the two scales, where dispersive flux and reactive source computations from micro- to macro-scale are carried on without any upscaling assumption.

Validation of the hybrid numerical scheme is performed in those regimes where upscaling assumptions hold.

Also, effects of Peclet (Pe) and Damkohler (Da) numbers are thoroughly investigated for those regimes where localized reactions and/or strong advection render homogeneized equations an inadequate descriptor of pore-scale processes.