

Hybrid multiscale model for evolving porous media

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Geological and engineered media are characterized by heterogeneity at multiple scales such that porosity is often distributed over a range of spatial scales. Pore-scale models make it possible to capture processes at the scale of individual pores but are computationally expensive for the simulation of large domains. Darcy-scale models are routinely used for efficient simulation of domains of any size. Multiscale models that combine pore- and Darcy-scale descriptions provide a reasonable compromise between the fine process-resolution of pore-scale models and the computational advantages of Darcy-scale models.

Reactions driven by the introduction of a fluid out of equilibrium with the native material result in the physical evolution of the media. This evolution may in turn alter the balance between the transport processes.

Here we build on previously developed hybrid model for the simulation of reactive transport in multiscale media [1] to include the evolution of the media. The model is composed of pore-scale and Darcy-scale sub-domains that make up the entire medium. The two sub-problems are solved sequentially by exchanging concentrations and fluxes at their interface. The evolution of the Darcy-scale domain is captured with porosity changes, while that of the pore-scale domain with the evolution of the interface.

We use the simulation of alteration of wellbore cement by CO₂ as an example to demonstrate the use of the model. We build on the conceptual model and simulations of [2] to construct a multiscale domain, where a fracture serves as a fast flow conduit for a CO₂-rich fluid, which diffuses into and alters the cement. The fracture is conceptualized as a pore-scale domain, and the cement as a Darcy-scale domain where reaction-diffusion controls the evolution.

[1] Molins et al (2019). Multi-scale Model of Reactive Transport in Fractured Media: Diffusion Limitations on Rates. *Transp. Porous Media*. 10.1007/s11242-019-01266-2

[2] Li et al. (2017). Incorporating Nanoscale Effects into a Continuum-Scale Reactive Transport Model for CO₂-Deteriorated Cement. *Environ. Sci. Technol*, 51(18), 10861–10871. 10.1021/acs.est.7b00594