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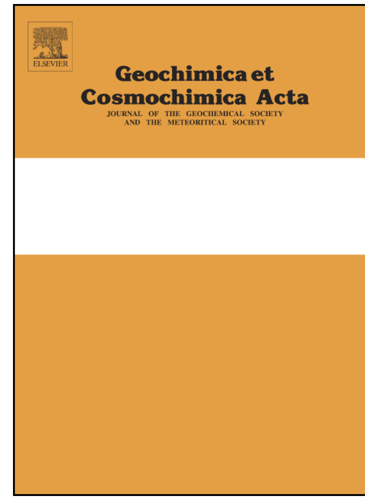

A new pore-scale model for linear and non-linear heterogeneous dissolution, precipitation and sorption reactions

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A new pore-scale model for linear and non-linear heterogeneous dissolution, precipitation and sorption reactions

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Abstract

Pore-scale processes exert a strong control on the transport of reactants in porous media at the continuum scale. As such, pore-scale numerical models can offer a more quantitative understanding of the coupling between transport and reaction and yield parameterized constitutive equations to introduce pore-scale corrections into macroscopic (continuum) reactive transport models.

In the present study, we present a new pore-scale model for the advection and diffusion of reactants in porous media with complex topologies. The model is based on the lattice Boltzmann method and couples a fluid flow solver to an optimal advection-diffusion transport model. Internal solid-fluid boundaries (grain boundaries) are explicitly part of the numerical domain, which allows the algorithm to solve for surface reactions independently from the surface shape and orientation of the grains. Thus, the approach is well suited for the treatment of heterogeneous reactions in complex pore structures.

We present single and multispecies reactive transport applications of the model. In the first application we study the permeability change of a porous medium associated with a given porosity change during dissolution and precipitation using linear reaction kinetics. We show that, for a given porous medium, the correlation between porosity and permeability changes depends on the transport regime (the ratio of advective to diffusive transport) and the reaction rate. Finally, we carry out simulations of multispecies reactive trans-

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