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A pore-scale lattice Boltzmann model for solute transport coupled with heterogeneous surface reactions and mineral dissolution

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In this paper, we propose a pore-scale lattice Boltzmann model to treat heterogeneous surface reactions coupled with mineral dissolution. The primary innovation lies in the transformation of surface reactions, originally treated as boundary conditions, into volume source terms through dimensionality augmentation within the framework of sharp liquid-solid interfaces. This significantly simplifies the implementation, particularly for reactions occurring in porous media with intricate geometric structures. Several benchmark tests were performed to validate the accuracy of this model, including a reaction-diffusion problem in a rectangular domain, a two-dimensional reaction and dissolution of a circular grain, as well as a three-dimensional calcite crystal dissolution in a micro-channel. All the obtained simulation results agree well with the reference solutions. In addition, a dissolution problem in a three-dimensional porous meida bulit with the sandpack is then investigated. Cases with different Peclet numbers (Pe) and Damkohler numbers (Da) were simulated, and five dissolution modes were obtained, which were finally summarized in a diagram of Pe and Da.

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Primary authors: LONG, Ju (King Abdullah University of Science and Technology); Prof. YAN, Bicheng (Los Alamos National Laboratory); Prof. SUN, Shuyu (King Abdullah University of Science and Technology (KAUST))

Presenter: LONG, Ju (King Abdullah University of Science and Technology)

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