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A modified Lattice Boltzmann model for pore-scale simulation of desorption process at surface water-groundwater interface

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A pore-scale numerical model is introduced to simulate the desorption process at surface water-groundwater interface. The Navier-Stokes equations for fluid and Advection-Diffusion equation for scalar transport are solved by Lattice Boltzmann Method (LBM). In previous studies, the macroscopic desorption kinetic equations are usually applied as a boundary condition. However, it may be problematic for pore-scale simulation since most desorption kinetic equations are fitted from macroscopic global variables. We avoid this problem by discretizing the particle surface into a large number of adsorption sites to mimic the microscopic desorption process. The state of each adsorption site follows the Langmuir's theory. Furthermore, benefiting from the mesoscopic inherent of the LBM, the total number of adsorbate which really contacted with the particle surface can be calculated rather than the local concentration. The predicted desorption Isotherm and concentration profile match well with theoretical solutions and experimental data. By using presented model, we find that the desorption process at surface water-groundwater interface shows a complex response to surface water flow.