

MACROSCOPIC REACTIVE TRANSPORT FROM PORE-SCALE SIMULATION

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Mixing of flowing fluids of non-uniform velocities in porous media coupled with a chemical reaction is a process that commonly occurs in contaminant transport in subsurface waters. Structural heterogeneity of porous media and spatially varying reaction rates pose major problems in obtaining an accurate description of the contaminant fate in subsurface.

We simulate reactive transport at macroscopic scale (scale of thousands of pores) by using a particle-tracking random-walk algorithm that accounts for micro-scale (single pore scale) mechanisms of diffusion, advection and chemical reaction. We use pore-scale model with the geometry and topology based on the networks extracted from the micro CT images of sandstone core samples. We study spatial and temporal probability density functions of tracer particles by using a Lagrangian pore-scale network model that incorporates flow, diffusion and chemical reaction in network lattices.

We show that the structurally and chemical reaction driven heterogeneity results in the reactive transport being anomalous or non-Fickian. We address the question on the nature of reactive transport in natural systems where the structural heterogeneities at the larger scales will significantly increase the range of velocities in the reservoir, thus significantly delaying the asymptotic approach to Gaussian behaviour.