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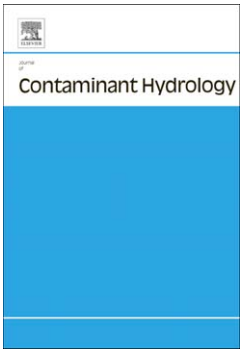

Predictions of Dynamic Changes in Reaction Rates as a Consequence of Incomplete Mixing Using Pore-scale Reactive Transport Modeling on Images of Porous Media

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ACCEPTED MANUSCRIPT

Title: Predictions of Dynamic Changes in Reaction Rates as a Consequence of Incomplete Mixing Using Pore-scale Reactive Transport Modeling on Images of Porous Media

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Abstract

We present a pore-scale model capable of simulating fluid/fluid reactive transport on images of porous media from first principles. We use a streamline-based particle tracking method for simulating flow and transport, while for reaction to occur, both reactants must be within a diffusive distance of each other during a time-step. We assign a probability of reaction (P_r), as a function of the reaction rate constant (k_r) and the diffusion length. Firstly, we validate our model for reaction against analytical solutions for the bimolecular reaction (A + B → C) in a free fluid. Then, we simulate transport and reaction in a beadpack to validate the model through predicting the fluid/fluid reaction experimental results provided by Gramling et al. (2002). Our model accurately predicts the experimental data, as it takes into account the degree of incomplete mixing present at the sub-pore (image voxel) level, in contrast to advection-dispersion-reaction equation (ADRE) model that over-predicts pore-scale mixing. Finally, we show how our model can predict dynamic changes in the reaction rate accurately accounting for the local geometry, topology and flow field at the pore-scale. We demonstrate the substantial difference between the predicted early-time reaction rate in comparison to the ADRE model.

Keywords: Fluid/fluid, reactive transport, pore-scale, micro-CT image, mixing, reaction rate.

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