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Modeling reactive transport with particle tracking and kernel estimators

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Groundwater reactive transport models are useful to assess and quantify the fate and transport of contaminants in subsurface media and are an essential tool for the analysis of coupled physical, chemical, and biological processes in Earth Systems. Particle Tracking Method (PTM) provides a computationally efficient and adaptable approach to solve the solute transport partial dierential equation. On a molecular level, chemical reactions are the result of collisions, combinations, and/or decay of dierent species. For a well-mixed system, the chemical reactions are controlled by the classical thermodynamic rate coefcient. Each of these actions occurs with some probability that is a function of solute concentrations. PTM is based on considering that each particle actually represents a group of molecules. To properly simulate this system, an infinite number of particles is required, which is computationally unfeasible. On the other hand, a finite number of particles lead to a poor-mixed system which is limited by diffusion. Recent works have used this effect to actually model incomplete mixing in naturally occurring porous media. In this work, we demonstrate that this effect in most cases should be attributed to a defficient estimation of the concentrations and not to the occurrence of true incomplete mixing processes in porous media. To illustrate this, we show that a Kernel Density Estimation (KDE) of the concentrations can approach the well-mixed solution with a limited number of particles. KDEs provide weighting functions of each particle mass that expands its region of influence, hence providing a wider region for chemical reactions with time. Simulation results show that KDEs are powerful tools to improve state-of-the-art simulations of chemical reactions and indicates that incomplete mixing in diluted systems should be modeled based on alternative conceptual models and not on a limited number of particles.