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Reactive transport in porous media with local mixing limitation: A Lagrangian modeling approach

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Hydrological models are unable to fully resolve subsurface flow and transport down to the microscale. Instead, modelers usually work with upscaled flow and transport properties that represent the behavior of the system at a given coarse scale. While this approach is justified from a practical standpoint, it disregards the local heterogeneity of porous media flows, which tend to produce mixing-limited reactive transport behaviors that cannot be captured by classical modeling approaches. While some innovative methods have been suggested in the past in order to address this problem, none of them has proposed a mathematical formulation which can potentially reproduce the generation, transport and decay of local concentration fluctuations and their impact on chemical reactions, for general initial and boundary conditions. Here, we propose a Lagrangian approach based on the random motion of fluid particles that locally mix following a Multi-Rate Interaction by Exchange with the Mean (MRIEM) formulation. Concentration fluctuations in the proposed model display the typical behavior associated to transport in porous media with mixing-limited conditions. Experimental results of reactive transport are successfully reproduced by the model.