Title: Modeling multicomponent reactive transport with particle tracking and smoothing techniques

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Abstract.

Major challenges associated with modeling reactive transport in naturally heterogeneous porous media include the incorporation of the joint effect of physical and biochemical heterogeneity into geochemical transport models. Available codes typically suffer from computational burden and numerical problems stemming from the required accurate description of heterogeneity in complex geochemical systems. Particle tracking methodologies to simulate transport constitute an attractive alternative for their computational efficiency and absence of numerical dispersion. Yet, problems stemming from the reconstruction of concentrations from particle distributions have typically prevented its use in reactive transport problems. The numerical problem mainly arises from the need to first reconstruct the concentrations of species/components from a discrete number of particles, which is an error prone process, and then computing a spatial functional of the concentrations and/or its derivatives (either spatial or temporal). Errors are then propagated, so that common strategies to reconstruct this functional require an unfeasible amount of particles when dealing with reactive transport problems. We provide a methodology to automatically reconstruct an optimal functional that renders particle tracking techniques the capability to be potentially coupled to any existing geochemical transport code. The method is used to analyze the effects of mixing-limited dynamics on the evolution of a serial reaction chemical system at the field scale.