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Adapting particle methods to model the dynamics of concentration gradients and chemical reactivity under advective diffusive transport conditions

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Abstract

Concentration organization and dynamics in heterogeneous porous media are key physical factors driving chemical reactivity. At equilibrium, reactivity depends not only on the concentration distribution but also on concentration gradients. As high and low values of concentration and concentration gradient do not superpose, we derive a transport equation for the concentration gradients and set up an adapted particle method to approach them numerically. Particles dynamically optimize their organization to provide highly accurate concentration gradients. The global strategy combining separate particle methods for the concentration and its gradient gives optimal predictions of reactivity.

Keywords: *transport equation concentration gradient particle methods diffusion velocity method.*