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Can we use mass transfer models to upscale non-reactive solute transport phenomena in heterogeneous formations?

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We evaluate the use of mass transfer models to upscale non-reactive solute transport phenomena in heterogeneous formations. Instead of using mass transfer equations to describe pore-scale chemical and/or physical non-equilibrium, mass transfer processes are intended to characterize the mass exchange between highly mobile and less mobile zones at the Darcy-scale. The study considers a modeling framework in which point measurements of hydraulic conductivity are required to be transferred to larger homogenized blocks. Thus, by construction, the upscaled flow model can only partially describe the velocity fluctuations occurring at the point scale. The flow model simplification is in turn compensated by incorporating mass transfer processes in the conceptual model of transport. Starting from a high-resolution description of hydraulic conductivity, we upscaled the flow problem by means of the Laplacian method with skin. Equivalent block transport and mass transfer parameters are then estimated by curve-fitting tracer test breakthrough curves using an inverse optimization technique. Performance assessment of the power-law mass transfer function is presented in this paper. To achieve this, solute transport is solved at different support scales. The fine scale solution constitutes the reference solution, which is compared to the upscaled model. Simulation of solute transport with mass transfer processes is based on the implementation of the multirate mass transfer model into random walk particle tracking presented by Salamon *et al.* [2006].