



Modeling transport at large scale using upscaled mass transfer models

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The usual observation of anomalous (non-Fickian) transport in the field, manifested by peaked concentration profiles with pronounced tailing, has questioned the use of the classical advection-dispersion equation (ADE) to model transport phenomena at the usual computational scale of a numerical model. In this context, we evaluate the use of (multi-rate) mass transfer models as the constitutive transport model for upscaling. Solute transport at computational scale consists in a phenomenological model based on memory functions that are used to represent the unresolved processes taking place within each homogenized block of the numerical model. The parameter values associated with the memory functions are determined by transferring the small-scale information on aquifer attributes into the computational scale defined by the numerical model discretization. Performance assessment of the alternative transport equation is achieved by comparing transport simulations of a non-reactive solute plume at two different support scales. The results demonstrate that the constitutive transport model can reproduce the mean behavior of the main features associated with the breakthrough curves.