The impact of mass transfer limitations and heterogeneity contrasts on the parameterization of longitudinal dispersion in numerical models

Lee, Jonghyun; Rolle, Massimo; Kitanidis, Peter

Publication date:
2017

Document Version
Peer reviewed version

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Presenter: Massimo Rolle
Contact Author: Massimo Rolle

AUTHORS

Jonghyun Lee [1], Massimo Rolle [2], Peter Kitanidis [3]

1 Stanford University, Stanford, US
2 Technical University of Denmark, Lyngby, DK
3 Stanford University, Stanford, US

ABSTRACT

A challenge in modeling solute transport in groundwater is how to parameterize hydrodynamic dispersion and which values to assign to coefficients in the blocks representing grid cells of a numerical model. Actual geologic formations are heterogeneous at all scales but numerical models resolve only larger scale heterogeneity by considering blocks with different parameters, while heterogeneity at scales smaller than the size of blocks is not explicitly resolved. Dispersion coefficients originate from the joint variability of velocities and solute concentrations at the small grain scale and at heterogeneity scales that are not resolved in the continuum description of solute transport within a given block.

In this study we focus on the longitudinal dispersion coefficient and, starting from accurate local scale description of solute transport, we apply an Eulerian approach for computing the values of longitudinal dispersion coefficient to be assigned to numerical models' blocks. The method is valid under conditions of physical equilibrium for which dispersion is approximately Fickian (i.e., the dispersive flux is proportional to the gradient of the resolved concentration). The approach requires the solution of a steady-state advection-dispersion equation; it is computationally efficient, and applicable to any heterogeneous hydraulic conductivity field. In this work we consider binary heterogeneous media with a permeable matrix and distributed low-permeability inclusions. Numerical experiments where performed in blocks containing the same volume of low-permeability material but with different orientation, elongation and hydraulic conductivity contrast of the inclusions with respect to the permeable matrix (s2lnK=0.2-4.6). Multi-tracer simulations considering solutes with different aqueous diffusion coefficient were performed in a range of seepage velocity values spanning the conditions typical of groundwater transport problems. The results demonstrate the critical role of the interplay between advection and diffusion, as well as the importance of the heterogeneity contrast. In some cases characterized by low permeability contrast, small inclusions and fast seepage velocity, computed longitudinal dispersion coefficients for the considered blocks can be captured satisfactorily by the linear Scheidegger parameterization, using a constant dispersivity. However, when diffusive mass transfer plays an important role, non-linear and compound-specific parameterizations should be used to accurately calculate longitudinal dispersion coefficients in discretized numerical models. Implications of these findings for mixing-controlled reactive transport problems will also be discussed.

GRAPHICS