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Application of block-scale effective dispersion to reactive transport simulations in groundwater

Paulo Herrera (1), Joaquin Cortinez (1), and Albert Valocchi (2)

(1) Department of Civil Engineering, U. Chile (pherrera@ing.uchile.cl), (2) Department of Civil and Environmental Engineering, U. Illinois at Urbana-Champaign (valocchi@illinois.edu)

In the groundwater literature, macrodispersion has traditionally been derived and applied to account for plume spreading –i.e. deformation of the water volume that contains solute mass- due to the overall heterogeneity of aquifers. Several experimental and numerical studies have verified that the use of a macrodispersion coefficient within an advection-dispersion equation can reproduce plume spreading in mildly heterogeneous aquifers. More recently, there have been new extensions to the macrodispersion theory to separately account for block-scale filtering effects due to the use of finite-size numerical grids, and for deriving effective macrodispersion coefficients to account for solute mixing and dilution.

We combine the concepts of block-scale dependent and effective dispersion to account for the effect of unresolved subgrid-scale heterogeneity on synthetic numerical simulations of a mixing controlled bimolecular reaction. We demonstrate that by using a time-dependent effective block-scale dispersion coefficient we are able to reproduce overall reaction rates for different scenarios defined according to parameters such as: grid size, Peclet number, aquifer heterogeneity, etc. Moreover, we verify that for long-times the block-scale effective dispersion coefficient that reproduces mixing is equal to the previously derived block-scale dispersion coefficient that reproduces spreading. Given that the block-scale dispersion coefficient is similar to the traditional macrodispersion coefficient in the limit of infinitely large block-sizes, we conclude that the block-scale time-dependent dispersion coefficient constitutes a natural extension of the macrodispersion theory that provides a unified framework for numerical simulations of reactive transport in heterogeneous aquifers.