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A Lagrangian scheme to model subgrid-scale mixing in heterogeneous porous media

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Small-scale heterogeneity of permeability plays a major role in the spreading and mixing of contaminant plumes in groundwater systems. Spreading and mixing are interrelated because heterogeneity-induced spreading leads to the stretching of interfaces of the contaminant plume, while mixing across the interfaces is governed by local hydrodynamic dispersion. In many practical problems, mixing is the key process since it controls peak contaminant concentrations and overall rates of reaction during engineered or in-situ remediation. In spite of advances in high performance computing, it is still not possible to resolve all spatial heterogeneity scales in numerical simulation of conservative and reactive transport. We propose a Lagrangian numerical approach to implement closure models to account for subgrid-scale spreading and mixing in Darcy-scale numerical simulations of solute transport in mildly heterogeneous porous media. The novelty of the proposed approach is that it considers two different dispersion coefficients to account for advective spreading mechanisms and local scale dispersion. This technique considers fluid particles that carry solute mass and whose locations evolve according to a deterministic component given by the grid-scale velocity and a stochastic component that corresponds to a block-effective macro-dispersion coefficient. Mass transfer between particles due to local-scale dispersion is approximated by a meshless method.

Using results of benchmark numerical simulations, we demonstrate that the proposed approach is able to model subgrid-scale spreading and mixing provided there is a correct choice of block-scale dispersion coefficient. We assume for convenience the common adopted model that the hydraulic conductivity is a second-order stationary, log-normally distributed random field with exponential covariance. This allows use of the closed-form expressions for the block effective macro dispersion coefficient developed by Rubin and co-workers [1] for the case of small variance.
The presentation will be based on our recently published paper [2].

References

[1] Rubin, Y., Sun, A., Maxwell, R. & Bellin, A.: The concept of block effective macrodispersivity and a unified approach for grid-scale- and plume-scale-dependent transport, J. Fluid Mech., 395, 161–180, 1999.
[2] Herrera, P. A., J. M. Cortınez, and A. J. Valocchi (2017), Lagrangian scheme to model subgrid-scale mixing and spreading in heterogeneous porous media, Water Resour. Res., 53, 3302–3318, doi:10.1002/ 2016WR019994.

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