A MULTISCALE LAGRANGIAN APPROACH FOR THE NUMERICAL SIMULATION OF SOLUTE MIXING IN HETEROGENEOUS POROUS MEDIA

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Solute mixing in porous media is the result of transport processes that occur at multiple scales. From local-scale dispersion, that acts at the scale of pore throats; to variations in Darcy or macro-scale velocity, which produce solute spreading at the macro-scale. Furthermore, variations in macro-scale velocity may enhance the action of local-scale dispersion resulting in higher effective mixing rates.
We present a new multiscale Lagrangian approach to model mixing in numerical simulations that overcomes some of the issues with traditional models based on the advection-dispersion equation with a single dispersion coefficient. The proposed approach is based on the use of a multiscale particle method. Particles carry solute mass and their locations evolve according to a random walk particle tracking method that includes 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. Thus, mixing mechanisms that occur at different scales are represented by two different dispersion coefficients. This makes possible to study separately the effect of local-scale dispersion and solute spreading on solute mixing and reaction rates.
We demonstrate some of the advantages of the proposed scheme in a set of benchmark simulations that consider the transport of two chemical species that undergo a bimolecular chemical reaction.