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Filtered density function approach for reactive transport in groundwater

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Spatial filtering may be used in coarse-grained simulations (CGS) of reactive transport in groundwater, similar to the large eddy simulations (LES) in turbulence. The filtered density function (FDF), stochastically equivalent to a probability density function (PDF), provides a statistical description of the sub-grid, unresolved, variability of the concentration field. Besides closing the chemical source terms in the transport equation for the mean concentration, like in LES-FDF methods, the CGS-FDF approach aims at quantifying the uncertainty over the whole hierarchy of heterogeneity scales exhibited by natural porous media. Practically, that means estimating concentration PDFs on coarse grids, at affordable computational costs.

To cope with the high dimensionality of the problem in case of multi-component reactive transport and to reduce the numerical diffusion, FDF equations are solved by particle methods. But, while trajectories of computational particles are modeled as stochastic processes indexed by time, the concentration's heterogeneity is modeled as a random field, with multi-dimensional, spatio-temporal sets of indices. To overcome this conceptual inconsistency, we consider FDFs/PDFs of random species concentrations weighted by conserved scalars and we show that their evolution equations can be formulated as Fokker-Planck equations describing stochastically equivalent processes in concentration-position spaces. Numerical solutions can then be approximated by the density in the concentration-position space of an ensemble of computational particles governed by the associated Itô equations. Instead of sequential particle methods we use a global random walk (GRW) algorithm, which is stable, free of numerical diffusion, and practically insensitive to the increase of the number of particles.

We illustrate the general FDF approach and the GRW numerical solution for a reduced complexity problem consisting of the transport of a single scalar in groundwater. Randomness is induced by the stochastic parameterization of the hydraulic conductivity, characterized by short range correlations and small variance. The objective is to infer the statistics of the random concentration sampled at the plume center of mass, integrated over the transverse dimension of a two-dimensional spatial domain. The FDF problem is therefore formulated in a two-dimensional domain as well, one spatial dimension and one in the concentration space. Upscaled drift and diffusion coefficients describing the transport of the FDF in the physical space are estimated on single-trajectories of diffusion in velocity fields with short-range correlations, owing to their self-averaging property. The mixing coefficients describing the transport in concentration spaces are parameterized by the trend and the noise inferred from the statistical analysis of an ensemble of simulated concentration time series, as well as by the classical "interaction by exchange of the mean" (IEM) mixing model. A Gaussian spatial filter applied to a Kraichnan velocity field generator is used to construct CGS-FDF simulations. We obtain highly accurate solutions for the mean concentration. At moderately large times, we find that the cumulative distribution function converges to the reference Monte Carlo solution. Instead, the FDF itself agrees with the Monte Carlo results only at small times. The analysis of the CGS-FDF simulations indicates that an IEM mixing model with variable characteristic time parameter could improve the FDF results.