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Parameterization and Monte Carlo solutions to PDF evolution equations

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The probability density function (PDF) of the chemical species concentrations transported in random environments is governed by unclosed evolution equations. The PDF is transported in the physical space by drift and diffusion processes described by coefficients derived by standard upscaling procedures. Its transport in the concentration space is described by a drift determined by reaction rates, in a closed form, as well as a term accounting for the sub-grid mixing process due to molecular diffusion and local scale hydrodynamic dispersion. Sub-grid mixing processes are usually described by models of the conditionally averaged diffusion flux or models of the conditional dissipation rate. We show that in certain situations mixing terms can also be derived, in the form of an Itô process, from simulated or measured concentration time series.

Monte Carlo solutions to PDF evolution equations are usually constructed with systems of computational particles, which are well suited for highly dimensional advection-dominated problems. Such solutions require the fulfillment of specific consistency conditions relating the statistics of the random concentration field, function of both space and time, to that of the time random function describing an Itô process in physical and concentration spaces which governs the evolution of the system of particles. We show that the solution of the Fokker-Planck equation for the concentration-position PDF of the Itô process coincides with the solution of the PDF equation only for constant density flows in spatially statistically homogeneous systems. We also find that the solution of the Fokker-Planck equation is still equivalent to the solution of the PDF equation weighted by the variable density or by other conserved scalars.

We illustrate the parameterization of the sub-grid mixing by time series and the Monte Carlo solution for a problem of contaminant transport in groundwater. The evolution of the system of computational particles whose density approximates the concentration PDF is numerically modeled with a global random walk algorithm, highly accurate, stable and free of numerical diffusion.