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Review

Diffusion in random velocity fields with applications to contaminant transport in groundwater

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ABSTRACT

The process of diffusion in a random velocity field is the mathematical object underlying currently used stochastic models of transport in groundwater. The essential difference from the normal diffusion is given by the nontrivial correlation of the increments of the process which induces transitory or persistent dependence on initial conditions. Intimately related to these memory effects is the ergodicity issue in subsurface hydrology. These two topics are discussed here from the perspectives of Itô and Fokker–Planck complementary descriptions and of recent Monte Carlo studies. The latter used a global random walk algorithm, stable and free of numerical diffusion. Beyond Monte Carlo simulations, this algorithm and the mathematical frame of the diffusion in random fields allow efficient solutions to evolution equations for the probability density of the random concentration.

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1. Introduction

Stochastic modeling became a leading paradigm in studies of complex systems since several decades. Random media, random environments, or random fields are central topics for thousands of research papers in physics, technology, geophysics, and life sciences. For instance, a search for the topic "random media" in Web of Science (seen online in January 2014) returns 4110 results and 2073 average citations per year in the last two decades, with a strong increasing trend. A similar dynamics (3197 results with 1345 average citations per year) shows for the same period the topic "groundwater contamination", which is one of the investigation directions where the "randomness" paradigm is intensively used.

Mathematical models of transport in random environments (e.g. continuous diffusion processes with random coefficients or random walks with random jump probabilities [11]) are often used for phenomena which are not reproducible experimentally under macroscopically identical conditions or in cases where the incomplete knowledge of the physical parameters precludes deterministic descriptions. To the first class belongs the turbulence, characterized by an intrinsic randomness, which is modeled by random velocity fluctuations [47,49,78,109]. In plasma physics the turbulent state of the system of charged particles is described by random electric potentials and magnetic fields [6,7]. Transport in groundwater belongs to the second class. The way randomness enters modeling in hydrogeology is through stochastic parameterizations of incompletely known hydraulic conductivity fields which induce random Darcy velocity fields [25,44].

A common feature of transport processes in random environments is the apparent increase of the diffusion coefficients with the scale of observation. In hydrogeology, the increase from Darcy scale, to laboratory, and to field scale of the diffusion coefficients inferred from measurements through different approaches (by fitting concentrations with solutions of advection–diffusion equations, by computing spatial moments of tracer concentrations, or by analysis of concentration series recorded at different travel distances from the source) has been called "scale effect" [17,18,42]. Similar scale dependence characterizes the so called "running diffusion coefficient" in plasma physics [5] and the "turbulent diffusivity" in turbulence [79,109].

Another characteristic of transport in random media is the presence of various memory effects associated with the departure of the transport process from a genuine Gaussian diffusion. Memory effects manifested by non-Markovian evolution were explicitly associated with the stochastic nature of the environment in plasma physics [6]. In the frame of stochastic subsurface hydrology, the departure from Fickian, linear-time behavior of the second moment of the solute plume may be interpreted as a memory effect [88,104]. This type of memory effects is usually associated with Markovian diffusion processes and are omnipresent in stochastic models of transport in groundwater. The prototype memory-free process is the Wiener process with independent increments. Therefore, a direct quantification of such memory effects is provided by correlations of increments of the transport process [92].

The groundwater is contained in aquifer systems consisting of spatially heterogeneous hydrogeological formations. The scarcity of direct measurements of their hydraulic conductivity is compensated by spatial interpolations and empirical correlations, further modeled as space random fields [14]. The groundwater flow caused by piezometric pressure gradients is usually modeled by Darcy law for the filtration velocity in porous media and the randomness of the hydraulic conductivity induces the randomness of the flow velocity [25]. Contaminant solutes are transported by advection, diluted by diffusion and hydrodynamic dispersion, and undergo various chemical reactions. Under simplifying assumptions, also supported by experiments, the hydrodynamic dispersion is approximated as a Gaussian diffusion [84] and summing up the molecular diffusion at the pore-scale one arrives at a local scale diffusive model with diffusive flux governed by Fick's law [8]. Hence, the primary mechanism responsible for the fate of contaminants in groundwater can be described as a diffusion in random velocity fields.

Concentrations and transition probability densities of the diffusion in given realizations of the random velocity field are governed by parabolic partial differential equations local in time and space. However, in case of statistically non-homogeneous fields, theoretical investigations [71] and numerical simulations [72] show that the evolution of the ensemble average concentration is non-Fickian and has to be described by integro-differential equations non-local in both time and space. Non-locality also may occur in modeling the local dispersion. For instance, following the Mori–Zwanzig memory function formalism of the equilibrium statistical mechanics [19,22,120], Cushman and Ginn derived space–time nonlocal models for diffusion in porous media with hydraulic parameters displaying fractal character [20,21]. A model non-local in time but local in space is the "continuous time random walk" process, with uncorrelated polydisperse features consisting of a random walk with waiting times uniformly sampled from a probability distribution [46], which has been proposed by Berkowitz and Scher [9,10] to describe the behavior of the ensemble mean concentration. A comparative study of such non-local models is presented in a review paper by Neuman and Tartakovsky [73]. Since non-local and non-Fickian behavior may arise from either normal or anomalous local scale diffusion models, it is difficult to extract information on the true nature of the stochastic transport process from experiments and diffusion in random velocity fields remains competitive with respect to the other models analyzed in [73]. Moreover, if the hydraulic conductivity and the velocity field may be characterized by power-law correlations, the model of diffusion in random fields naturally leads to anomalous diffusive behavior of the transport process [39,92]. Estimates of the prediction errors [71,73] and ergodicity assessments [34,95] also can be obtained by comparing results for fixed realizations of the random field, corresponding to the observed transport process, to their ensemble averages. Last but not the least, the model of diffusion