Advances in Water Resources 119 (2018) 60–69

Contents lists available at ScienceDirect

Advances in Water Resources

journal homepage: www.elsevier.com/locate/advwatres

A coupled time domain random walk approach for transport in media characterized by broadly-distributed heterogeneity length scales

Tomás Aquino*, Marco Dentz

Spanish National Research Council (IDAEA – CSIC), 08034 Barcelona, Spain

ARTICLE INFO

Keywords:
Time domain random walk
Spatial heterogeneity
Stochastic modeling

ABSTRACT

We develop a time domain random walk approach for conservative solute transport in heterogeneous media where medium properties vary over a distribution of length scales. The spatial transition lengths are equal to the heterogeneity length scales, and thus determined by medium geometry. We derive analytical expressions for the associated transition times and probabilities in one spatial dimension. This approach determines the coarse-grained solute concentration at the interfaces between regions; we derive a generalized master equation for the evolution of the coarse-grained concentration and reconstruct the fine-scale concentration using the propagator of the subscale transport mechanism. The performance of this approach is demonstrated for diffusion under random retardation in power-law media characterized by heavy-tailed lengthscale and retardation distributions. The coarse representation preserves the correct late-time scaling of concentration variance, and the reconstructed fine-scale concentration is essentially identical to that obtained by direct numerical simulation by random walk particle tracking.

1. Introduction

Physical and chemical heterogeneity, which often spans multiple scales, has important consequences for solute transport in natural and engineered media. It is well known that heterogeneity may lead to anomalous (non-Fickian) characteristics, even if the transport mechanism is advective or diffusive at smaller scales (Bouchaud and Georges, 1990; Comolli et al., 2016; Dentz et al., 2004; Havlin and Ben-Avraham, 1987; Klages et al., 2008). Upscaling transport dynamics is essential for understanding, and providing efficient methods for predicting, large-scale solute transport. This is particularly true in view of computational constraints and incomplete information about medium properties.

The continuous time random walk (CTRW) framework provides analytical and computational tools for describing transport by considering (conceptual) Lagrangian particles whose movement is characterized by spatial jumps and inter-jump waiting times (Berkowitz et al., 2006; Scher and Lax, 1973). The CTRW as an average transport framework encodes information about the variability in transport dynamics due to subscale heterogeneity through the statistical properties of transition times and distances. Derivation of CTRW-type large-scale descriptions typically requires averaging over an ensemble of medium, or heterogeneity, realizations (Berkowitz and Scher, 1997; Bouchaud and Georges, 1990; Comolli and Dentz, 2017; Dentz and Castro, 2009; Klafter and Silbey, 1980; Painter and Cvetkovic, 2005; Scher and Lax, 1973). Here, we use the term time domain random walk (TDRW) to refer to CTRW approaches which solve transport in single medium representations (Banton et al., 1997; Delay and Bodin, 2001; Dentz et al., 2012; James and Chrysikopoulos, 2001; McCarthy, 1993; Noetinger et al., 2016; Painter et al., 2008). Transport properties at a given spatial location are fixed, and a particle revisiting a location will sample the same properties.

We consider a one-dimensional medium characterized by a broad distribution of heterogeneity length scales and transport properties, as illustrated in Fig. 1. Specifically, we consider spatially variable advection and dispersion as a result of heterogeneous retardation and analyze dispersive trapping and regular dispersion as the small-scale transport mechanisms (Bouchaud and Georges, 1990). We construct a TDRW description with spatial transitions over the heterogeneity length scales and derive transition times and transition probabilities that encode the statistical properties of the subscale dynamics. These transition times and probabilities depend on the direction of the transition, resulting in a coupled TDRW model. This is in contrast to models where jump directions are uniformly distributed (Dentz et al., 2016; Massignan et al., 2014; Russian et al., 2017) and/or transition times are assumed to be independent of the jump direction (Dentz et al., 2012).

TDRW descriptions based on finite-volume discretizations of the advection–dispersion equation (ADE) do not resolve the particle position within a pixel or voxel. This gives rise to numerical dispersion, which can be addressed by refining the discretization (Russian et al.,

* Corresponding author.
E-mail address: tomas.aquino@idaea.csic.es (T. Aquino).

https://doi.org/10.1016/j.advwatres.2018.07.009
Received 12 May 2018; Received in revised form 16 July 2018; Accepted 17 July 2018
Available online 18 July 2018

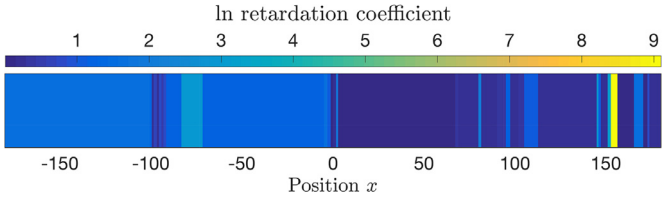

Fig. 1. Illustration of a one-dimensional medium with power-law-distributed region-dependent retardation coefficient and power-law-distributed region lengths.

2016). For transport in a medium whose properties are distributed on a hierarchy of macroscopic length scales, the subscale process needs to be accounted for in order to accurately represent the particle position and thus the concentration distribution. We derive a procedure for reconstructing the fine-scale concentration from the coarse-grained particle distribution obtained from the TDRW. In this sense, the resulting model represents a computationally efficient, particle-based, hybrid approach, in that it combines fast coarse-scale simulations with an efficient local reconstruction procedure.

2. Transport models

Solute concentration c $[ML^{-1}]$ for diffusive transport through a one-dimensional medium with trapping characterized by a position-dependent retardation coefficient θ $[-]$ obeys the Fokker–Planck equation (Bouchaud and Georges, 1990; Risken, 1996)

$$\frac{\partial c(x,t)}{\partial t} = -\frac{\partial}{\partial x}[v(x)c(x,t)] + \frac{\partial^2}{\partial x^2}[D(x)c(x,t)], \tag{1}$$

where $v(x) = v_0/\theta(x)$ $[LT^{-1}]$ is the transport velocity and $D(x) = \kappa/\theta(x)$ $[L^2T^{-1}]$, with κ the constant (molecular) diffusion coefficient and v_0 the constant flow velocity. Note that this is not a regular dispersion equation (except in the case of homogeneous retardation), because $\partial^2[D(x)c(x,t)]/\partial x^2 \neq \partial[D(x)\partial c(x,t)/\partial x]/\partial x$. Subsequently, we will call it the trapping equation. Equivalently, transport may be described by the Langevin equation for particle positions X,

$$dX(t) = v[X(t)]dt + \sqrt{2D[X(t)]dt}\,\xi(t), \tag{2}$$

where, for each time t, $\xi(t)$ is an independent Gaussian random variable with mean zero and unit variance. This equation is to be interpreted in the Itō sense (Kampen, 1992), and applies with independent ξ to each particle. It forms the basis for particle tracking random walk (PTRW) simulations, which we employ below to verify our results for the upscaled TDRW model. The Langevin description is Lagrangian, in the sense that it describes an ensemble of single-particle trajectories. Concentration, an Eulerian quantity measured at fixed spatial positions, corresponds to the probability density function (PDF) of Lagrangian particle positions scaled by the total mass. Throughout, we normalize concentrations to unit mass, so that the spatial integral of concentration is equal to 1 at all times. The Fokker–Planck equation for the PDF of particle position corresponding to 2 coincides with the trapping equation (Bouchaud and Georges, 1990).

For transport under spatially variable advection and regular dispersion (as opposed to trapping), the Fokker–Planck equation is the ADE,

$$\frac{\partial c(x,t)}{\partial t} = -\frac{\partial}{\partial x}[v(x)c(x,t)] + \frac{\partial}{\partial x}\left[D(x)\frac{\partial c(x,t)}{\partial x}\right]. \tag{3}$$

The corresponding Langevin equation is given by (Noetinger et al., 2016),

$$dX(t) = \left(v[X(t)] + \frac{dD[X(t)]}{dx}\right)dt + \sqrt{2D[X(t)]\,dt}\,\xi(t). \tag{4}$$

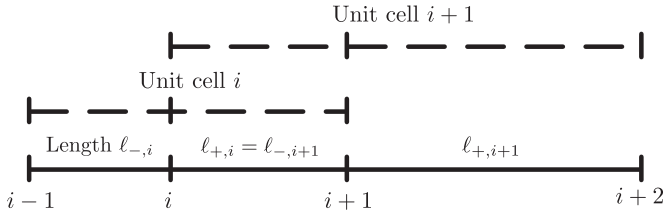

Fig. 2. Unit cells associated with nodes i and $i+1$.

The dynamics for spatially discontinuous dispersion can be integrated numerically using Eq. (2) along with a predictor–corrector method (LaBolle et al., 2000).

3. Coarse graining

We coarse-grain transport by considering a time domain random walk (TDRW) in a medium composed of segments characterized by a length and a constant retardation coefficient. We take particles to start at a given node between two segments; at each step n, particles wait for a random time T_n and then jump a length L_n to an adjacent node. We thus define our TDRW by the Lagrangian equations

$$X_{n+1} = X_n + L_n(X_n), \tag{5a}$$

$$T_{n+1} = T_n + \tau_n(X_n, L_n). \tag{5b}$$

For x the position of a node, let $\ell_+(x)$ and $\ell_-(x)$ be the lengths of the segments to its immediate right and left, respectively. Denote the probabilities of a jump to the right or left as $p_\pm(x)$. The jump length $L_n(x)$ is characterized by the probabilities $P\{L_n(x) = \pm\ell_\pm(x)\} = p_\pm(x)$. The transition times are given by $\tau_n(x,l) = \Theta(l)\tau_{n,+}(x) + \Theta(-l)\tau_{n,-}(x)$, where Θ is the Heaviside step function. We denote the PDFs of the travel times $\tau_{n,\pm}(x)$ given the direction of transition as $\psi_\pm(\cdot\,; x)$. We write also $D_\pm(x) = \kappa/\theta_\pm(x)$, where $\theta_\pm(x)$ are the retardation coefficients of the segments to the right and left of the node, and $v_\pm(x) = v_0/\theta_\pm(x)$ for the corresponding velocities.

3.1. First arrival times in the unit cell

We define a unit cell as composed of a central node and the two adjacent segments, as illustrated in Fig. 2. The transition probabilities $p_\pm$ represent the probabilities of a transported particle starting from the central node to first reach the node to the right or the node to the left. The $\psi_\pm$ represent the PDFs of the first arrival time to the corresponding node, given that node is reached first. Since the TDRW defined by Eq. (5) is Markovian in the transition n (no memory of previous transitions) and only allows transitions to adjacent nodes, this fully characterizes the system.

In order to find the first arrival time PDFs, we solve a Green function problem, for Eq. (1) for the trapping problem and Eq. (3) for the dispersion problem, with absorbing boundary conditions at the outer edges and a pulse initial condition of unit mass at $x = 0$. We choose a coordinate system such that $x = 0$ corresponds to the central node, and the edges are located at $-\ell_- < 0$ and $\ell_+ > 0$. The boundary and initial conditions for the Green function (i.e., concentration propagator) g are then

$$g(-\ell_-, t) = g(\ell_+, t) = 0, \quad g(x,0) = \delta(x), \tag{6}$$

where $\delta(\cdot)$ is the Dirac delta. Solutions can be written in the form

$$g(x,t) = g_-(x,t)\Theta(-x) + g_+(x,t)\Theta(x). \tag{7}$$

The continuity condition for $g(x,t)$ at the interface at $x = 0$ is obtained from the requirement that concentration be integrable anywhere in the unit cell. This implies for the trapping problem that

$$D_- g_-(0,t) = D_+ g_+(0,t). \tag{8}$$