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Characterization of mixing and spreading in a bounded stratified medium

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Matheron and de Marsily [Matheron M, de Marsily G. Is the transport in porous media always diffusive? A counter-example. Water Resour Res 1980;16:901–17] studied transport in a perfectly stratified infinite medium as an idealized aquifer model. They observed superdiffusive solute spreading quantified by anomalous increase of the apparent longitudinal dispersion coefficient with the square root of time. Here, we investigate solute transport in a vertically bounded stratified random medium. Unlike for the infinite medium at asymptotically long times, disorder-induced mixing and spreading is uniquely quantified by a constant Taylor dispersion coefficient. Using a stochastic modeling approach we study the effective mixing and spreading dynamics at pre-asymptotic times in terms of effective average transport coefficients. The latter are defined on the basis of local moments, i.e., moments of the transport Green function. We investigate the impact of the position of the initial plume and the initial plume size on the (highly anomalous) pre-asymptotic effective spreading and mixing dynamics for single realizations and in average. Effectively, the system "remembers" its initial state, the effective transport coefficients show so-called memory effects, which disappear after the solute has sampled the full vertical extent of the medium. We study the impact of the intrinsic non-ergodicity of the confined medium on the validity of the stochastic modeling approach and study in this context the transition from the finite to the infinite medium.

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1. Introduction

Transport in stratified media has been frequently studied in the groundwater literature as a model for transport in geological media. Natural sandy aquifers often exhibit geological and geostatistical stratification characterized by a much larger horizontal than vertical correlation length (see, e.g. [2] and literature therein). In the limiting case of infinite correlation length in the horizontal direction, the hydraulic conductivity varies only along the vertical. Following the deterministic work of Marle et al. [3], Matheron and de Marsily [1] studied this perfectly stratified medium as an idealized aquifer model. They found that the apparent longitudinal dispersion coefficient grows superdiffusively with the square root of time and used this result to demonstrate that transport in porous media is not always diffusive. Transport in an infinite perfectly stratified random medium has been investigated extensively (e.g. [4–11]) using stochastic modeling as a systematic means to quantify the impact of spatial heterogeneity on large scale transport. The latter has been studied in terms of the average solute distribution density and its moments, its spatial and temporal moments as well as in terms of (apparent) longitudinal dispersion coefficients.

The superdiffusive growth of the apparent longitudinal dispersion coefficient is caused by strong spatial correlation as quantified by the Lagrangian velocity correlation (e.g. [12,13]). These aspects of transport in stratified flows have been extensively studied in the physics literature (e.g. [14–17]).

In contrast to the unbounded stratified medium, for which transport is superdiffusive for all times, for a vertically (i.e., transverse to the direction of stratification) bounded medium, transport becomes eventually Gaussian and can be completely characterized by a constant macrodispersion or "Taylor dispersion-type" coefficient. Several authors have addressed the issue of enhanced dispersion and effective transport dynamics for bounded stratified random media and shear flows in general (e.g. [2,18–21]). Taylor [22] was the first to quantify enhanced solute dispersion in the parabolic (stratified) Hagen–Poiseuille flow through a tube by the well known Taylor dispersion coefficient

$$D^{*} \propto \frac{a^2 U^2}{D_{\mathrm{T}}}, \tag{1}$$

where a is a measure for the vertical extent of the flow domain, U the average flow velocity and D_{T} the transverse local dispersion coefficient, i.e. the transverse component of the (constant) dispersion tensor at local scale. The Taylor dispersion coefficient (1) reflects the mechanism that leads to enhanced spreading and mixing in stratified flows, namely, the solute's sampling of the vertical velocity contrast (U^2) by local transverse dispersion (D_{T}). The process is controlled by the dispersion time scale τ_{D}

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$$\tau_D = \frac{a^2}{D_T}, \tag{2}$$

which measures the time for the solute to sample the whole vertical velocity contrast. For times large compared to the dispersion time scale, $t \gg \tau_D$, the Taylor dispersion coefficient D^* quantifies both large scale spreading and mixing as well as the evolution of the solute concentration.

In hydrological applications, however, this dispersion time scale can be large (of the order of 10^3 years). At the relevant pre-asymptotic times, the constant Taylor or macrodispersion coefficient overestimates actual solute spreading and mixing. For risk assessment studies that focus on the maximum extent of a contaminant plume, macrodispersion gives simulates a worst case scenario and maybe the observable of choice. If one is interested in remediation strategies relying on the mixing of contaminated water with an injected reactant, the correct quantification of the pre-asymptotic mixing mechnisms is mandatory in order to be able to realistically assess the efficiency of the remediation strategy. Macrodispersion simulates to high a mixing efficiency and can significantly overestimate the performance of a remediation strategy.

At pre-asymptotic times, i.e., for times smaller than τ_D, solute spreading and mixing is controlled by local transverse dispersion, which activates the vertical velocity contrast as a macroscopic spreading and mixing mechanisms. As outlined in [23], transverse dispersion mixes the solute vertically. The velocity contrast experienced by the solute through vertical mixing stretches the plume and increases the plume surface but not the volume occupied by the solute, which is termed spreading [23]. Transverse dispersion then again leads to vertical mass exchange between the solute layers and smoothes concentration contrasts out, which leads to large scale mixing.

Here we investigate these mechanisms for a stratified random medium in terms of suitably defined second centered moments of the solute plume. This analysis is based on the moments of the transport Green function, i.e., the solute distribution that evolves from a point-like initial distribution. The latter allows for the construction of observables that measure spreading and/or mixing of the solute. Many studies of solute dispersion in single realization focus on the vertically averaged (over the directions perpendicular to the direction of stratification) solute concentration and in stochastic frameworks on ensemble averaged concentrations. The vertically averaged solute concentration quantifies (advective) solute spreading within the initial plume [24], the ensemble averaged concentration quantifies an artificial spreading effect due to sample to sample fluctuations of the plume's center of mass from realization to realization [25]. While for transport in heterogeneous media these fluctuations vanish in average for time large compared to the dispersion scale [26], for an infinite stratifies random medium they persist [10]. Furthermore, averaging over a large initial plume or stochastic averaging wipes out possible memory effects that account for the impact of the initial position or initial plume size on the effective transport behavior. We study these mechanisms systematically for single realizations and in stochastic average for confined stratified media using explicit analytical expressions and numerical random walk simulations. We discuss the stochastic approach for such confined scenarios and the impact of finite size effects on the ergodicity of transport.

In Section 2, we present the specific aquifer model under consideration, which is characterized by a linear covariance function for the conductivity in vertical direction. Section 3 introduces the concepts and defines the transport coefficients used to investigate the different mechanisms described above. This section presents analytical and numerical solution methods axial moment equations and random walk simulations, respectively. We derive explicite analytical solutions for the ensemble averaged transport coefficients. Section 4 applies these concepts and methods for the systematic analysis of mixing and spreading, Section 5 concludes the paper.

2. Model

We study transport of a conservative solute in a confined horizontally stratified medium. The d-dimensional flow and transport domain, denoted by Ω^d, is assumed to be of infinite extension at least in the one-direction and finite only in one of the transverse directions.

2.1. Flow and transport in stratified media

Flow through a stratified porous medium is characterized by the Darcy equation (e.g. [27])

$$\mathbf{u}(\mathbf{x}) = -\frac{K(\mathbf{y})}{\phi}\nabla h(\mathbf{x}), \tag{3}$$

where $\mathbf{u}(\mathbf{x})$ is the pore velocity, ϕ is the constant porosity, $\mathbf{x}$ is the position vector in Ω^d and $\mathbf{y} = (x_2, \ldots, x_d)^T$ is the position vector in the $(d-1)$-dimensional subdomain Ω, with $\Omega^d = \Omega \times \mathbf{R}$. In the following, for simplicity constant porosity is set to 1. The hydraulic conductivity is denoted by $K(\mathbf{y})$ and varies only in Ω, $h(\mathbf{x})$ is the hydraulic head. The flow is driven by a constant head gradient $\mathbf{J}$, which is aligned with the direction of stratification, $\mathbf{J} = -J\mathbf{e}_1$, where $\mathbf{e}_1$ is the unit vector in one-direction. Together with the incompressibility condition $\nabla \cdot \mathbf{u}(\mathbf{x}) = 0$, this boundary condition leads to the exact solution (e.g. [11])

$$\mathbf{u}(\mathbf{x}) = u(\mathbf{y})\mathbf{e}_1 = K(\mathbf{y})J\mathbf{e}_1. \tag{4}$$

Advective–dispersive transport of a conservative solute in the stratified flow field (4) is given by

$$\frac{\partial c(\mathbf{x},t)}{\partial t} + u(\mathbf{y})\frac{\partial c(\mathbf{x},t)}{\partial x_1} - \nabla\mathbf{D}\nabla c(\mathbf{x},t) = 0. \tag{5}$$

The (constant) local dispersion tensor $\mathbf{D}$ is assumed to be diagonal, $D_{ij} = \delta_{ij}D_{ij}$ with $D_{11} = D_L$ and $D_{ii} = D_T$ for $i > 1$.

As initial condition, we consider an instantaneous solute injection at time $t = 0$

$$c(\mathbf{x}, t = 0) = \rho(\mathbf{x}), \tag{6}$$

where the initial distribution $\rho(\mathbf{x})$ is normalized to one. As the stratified flow velocity is divergence-free, this normalization is conserved for all times. We study transport of a solute evolving from a point-like injection and from an extended source perpendicular to stratification. Both initial conditions will be described in the following. The boundary conditions for $c(\mathbf{x},t)$ are

$$\lim_{x_1\to\pm\infty} c(\mathbf{x},t) = 0, \quad \mathbf{n}\cdot\nabla c(\mathbf{x},t)|_{\mathbf{x}\in\partial\Omega^d} = 0, \tag{7}$$

where $\partial\Omega^d$ is the boundary of the transport domain Ω^d, and $\mathbf{n}$ is the outward pointing unit vector perpendicular to the domain boundaries.

According to the Duhamel principle, the concentration distribution $c(\mathbf{x},t)$ can be written as

$$c(\mathbf{x},t) = \int_{\Omega^d} d\mathbf{x}'\rho(\mathbf{x}')g(\mathbf{x},t|\mathbf{x}',0), \tag{8}$$

where the Green function $g(\mathbf{x},t|\mathbf{x}',t')$ solves the advection–dispersion equation (5) for $\rho(\mathbf{x}) = \delta(\mathbf{x}-\mathbf{x}')$ and the boundary conditions (7).

2.2. Stochastic model

We use a stochastic modeling approach to account for the impact of spatial heterogeneity on the effective large scale transport

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