Advances in Water Resources 121 (2018) 57–67

Contents lists available at ScienceDirect

Advances in Water Resources

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

A simple velocity random-walk model for macrodispersion in mildly to highly heterogeneous subsurface formations

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ARTICLE INFO

Keywords:
Macrodispersion
Transport uncertainty quantification
Non-Fickian transport
Random walk
Perturbation expansion
Langevin equation
Stochastic diffusion process
Periodic flow fields

ABSTRACT

Recently, we have analytically derived a temporal velocity random-walk model for macrodispersion or transport uncertainty quantification based on velocity statistics from classical first-order perturbation expansions. The applicability of these expansions is limited to mildly heterogeneous formations with log-conductivity variances $\sigma_Y^2 < 1$. In this work, we reformulate our model in order to account for velocity skewness and inter-component correlation that emerge as key drivers of non-Fickian dispersion at elevated heterogeneity levels σ_Y. Eventually, we arrive at a light-weight parametrization of macrodispersion that is consistent with our earlier formulation, but at the same time is applicable for formations with multi-Gaussian log-conductivity characterization of variable heterogeneity, i.e. σ_Y from 0 to 1 and beyond.

1. Introduction

Macrodispersion is the spreading of fluid or tracer particles resulting from spatial velocity differences (Gelhar, 1993, equation (5.1.10)). These differences may arise in an aquifer comprised of horizontal layers (Gelhar et al., 1979), just to give one possible scenario. For example in the well-documented Krauthausen tracer experiment, Vereecken et al. (2000, Section 5.1) extracted a vertical conductivity variogram with a clear nugget effect and roughly ten times smaller correlation length compared to its horizontal counterpart, which did not have a nugget. This behavior is indicative of a horizontal layer structure. Since the hydraulic conductivity $Y(\mathbf{x})$ is typically a spatially heterogeneous quantity (Gelhar, 1993, Fig. 1.3), the flow field in the different layers varies (Vereecken et al., 2000, Section 6.1). As a result, even though particles originate from the same vertical line in the aquifer, they will travel with different velocities in the layers, which leads to a horizontal spreading or dispersion. When focusing on the vertically averaged tracer concentration[1], macrodispersion is typically the dominant spreading mechanism compared to dispersion at the pore scale (see Dagan and Fiori, 1997 or Caroni and Fiorotto, 2005, Figs. 2, 5, and 6 with Péclet mostly >100 Rubin, 2003, Section 10.5.2).

Early attempts to model macrodispersion have focused on the advection–dispersion equation for the tracer concentration with time- or scale-dependent dispersivities (e.g., Dagan, 1987; de Dreuzy et al., 2007; Fernandez-Garcia et al., 2005; Salandin and Fiorotto, 1998; Silliman and Simpson, 1987). These dispersivities were studied experimentally for example by Silliman and Simpson (1987) or Fernandez-Garcia et al. (2005), derived analytically by means of low-order perturbation theory, e.g., by Dagan (1987) or Jaekel and Vereecken (1997), and numerically investigated for example by Salandin and Fiorotto (1998) or de Dreuzy et al. (2007) through Monte Carlo (MC) simulations. The numerical simulation studies revealed that deviations in velocity statistics and dispersivities between reference MC and perturbation theory become apparent for log-conductivity variances $\sigma_Y^2 > 1$. Deviations were mainly attributed to increasingly non-Gaussian velocity statistics that are induced by preferential flow paths or channels (Salandin and Fiorotto, 1998; Trefry et al., 2003) spanning over several correlation lengths l_Y of Y. More realistic stochastic models based on fluid or tracer particles have been developed since (e.g., Berkowitz et al., 2006; Le Borgne et al., 2008a; 2008b; Jenny et al., 2006; Kang et al., 2015; Meyer, 2017; Meyer and Saggini, 2016; Meyer and Tchelepi, 2010; Meyer et al., 2013) and were partly reviewed by Noetinger et al. (2016). While Berkowitz et al. (2006) promoted the versatile continuous time random walk (CTRW) framework—that was for example adapted by Le Borgne et al. (2008a,b) and Kang et al. (2015) for the description of diffusive/advective transport in heterogeneous porous media and advective transport in fractured media, respectively—our work has mainly focused on advective transport in two-dimensional multi-Gaussian fields with variable heterogene-

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[1] Groundwater wells can be viewed as vertical mixers over the different layers similar to a vertical average.

https://doi.org/10.1016/j.advwatres.2018.07.015
Received 6 November 2017; Received in revised form 22 June 2018; Accepted 24 July 2018
Available online 26 July 2018
0309-1708/

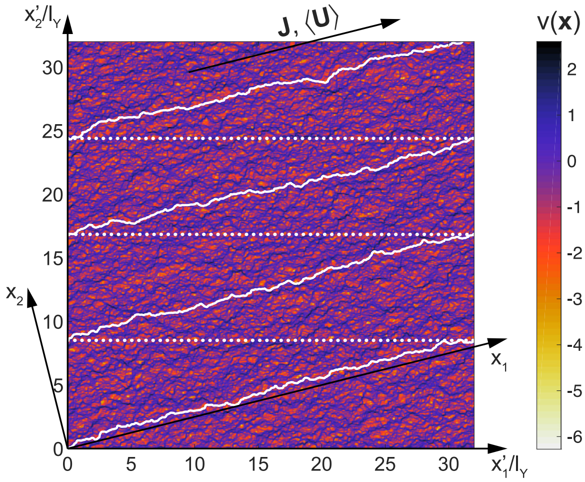

Fig. 1. Particle tracking in an exemplary doubly L-periodic flow field. The side length of the quadratic domain is $L = 32l_Y$ and $\sigma_Y = 2$. The particle pathline with periodic continuations is depicted with the white lines. The domain as well as the pathline coordinate systems are shown. The latter, i.e., $x_1 - x_2$, is aligned with the mean flow direction $\langle \mathbf{U} \rangle$ induced by the prescribed mean head gradient $\mathbf{J}$. The shading represents the distribution of $v(\mathbf{x}) = \log[|\mathbf{U}(\mathbf{x})|/U]$.

ity levels. Multi-Gaussian fields are widely applied and were recently found—in connection with ergodic plumes[2] and three-dimensional formations—to lead to similar dispersion behavior as more complex geostatistical models (Jankovic et al., 2017).

In our work (Meyer and Tchelepi, 2010; Meyer et al., 2013), we have systematically studied, similar to Trefry et al. (2003, Fig. 2) and Nowak et al. (2008), the increasingly complex velocity dynamics, which are at the heart of the non-Fickian transport behavior arising at elevated heterogeneity levels. These dynamics result from stagnant fluid motion in low-conductivity islands interrupted by intermittent high-velocity bursts induced by particle motion in high-conductivity channels. Moreover, we have investigated the applicability of temporal velocity random walks (RWs) as surrogate models for these dynamics, by systematically evaluating the Markov hypothesis for the Lagrangian velocity process (Meyer and Saggini, 2016). Velocity RW models were formulated (Meyer and Tchelepi, 2010; Meyer et al., 2013), that account for the velocity skewness and the complex temporal correlation behavior in the absence of pore-scale dispersion. The addition of pore-scale dispersion—which is typically accounted for in Lagrangian numerical schemes by Brownian motion (Salamon et al., 2006)—increases velocity de-correlation and promotes randomness, which seem to facilitate the formulation of stochastic models.

The previously outlined Lagrangian models are particularly useful in the context of reactive flows as showcased in the extensive work of Pope (2011) about flow and transport in turbulence. While fluid-phase reaction source terms can be incorporated in exact form and the effect of pore-scale dispersion on the mean concentration can be reflected by a Brownian motion in the particle position equation (Meyer et al., 2010, Eqs. (10) and (20)), mixing models are required to account for species mixing or dilution within fluid particles due to sub-Darcy or pore-scale effects (Meyer et al., 2010, Eq. (12); Suciu et al., 2015). Current research efforts focus on a better understanding of mixing in heterogeneous porous media (e.g., Aquino and Bolster, 2017; Le Borgne et al., 2013; Dentz et al., 2011; de Dreuzy et al., 2012; Lester et al., 2016).

Furthermore, the previously outlined Lagrangian models can be applied in the context of uncertainty quantification of subsurface flow and transport. Here, the different aquifer layers of the initial example translate into several probable scenarios of a shallow two-dimensional aquifer with uncertain transmissivity distribution[3]. Fluid particles now travel in different aquifer scenarios or realizations enabling the estimation of, e.g., the concentration mean/standard deviation distributions or the concentration probability density function (PDF). In our contributions (Dünser and Meyer, 2016; Meyer et al., 2013), we demonstrate the applicability of our stochastic models for highly non-stationary settings involving different transmissivity measurement configurations. From our model computations, transport predictions were obtained at a tiny fraction of the computational cost of standard MC (Meyer et al., 2013, Section 4.2.3).

During the review process, we were made aware of the percolation-based framework by Hunt and coworkers (Ghanbarian-Alavijeh et al., 2012; Hunt and Skinner, 2008). Here, similar to preferential flow paths that form at the Darcy-scale for σ_Y high, critical paths establish in strongly disordered pore networks. In connection with critical path analysis, Hunt and coworkers outline a model for dispersion phenomena in partly as well as fully saturated media with fractal pore-radius distributions and apply the model in a number of cases (Hunt and Sahimi, 2017). Certain model parameters are determined, for example in the saturated case, by fitting the particle arrival-time distribution for one medium size and by predicting subsequently arrival-times at other sizes (Hunt and Skinner, 2008).

Similarly, most of the previously cited RW modeling efforts rely on numerical model calibration: Le Borgne et al. (2008a,b) used numerical velocity transition matrices, while curve fits for drift and diffusion functions (corresponding to velocity transition moments) were applied in our work (Meyer and Tchelepi, 2010; Meyer et al., 2013). More recently, we have analytically derived these functions for temporal stochastic diffusion processes of fluid particles in mildly heterogeneous multi-Gaussian fields (Meyer, 2017). To this end, the Gaussian Lagrangian velocity statistics resulting from first-order perturbation theory (Dagan, 1985; Rubin, 1990) were used as a basis. In the present contribution, we reformulate the RW model derived from perturbation theory such that it becomes compatible with the non-Gaussian velocity statistics that emerge at increasing σ_Y. The reformulated RW model reduces for $\sigma_Y \to 0$ to its Gaussian origin from perturbation theory and is considerably simpler compared to our earlier efforts (Meyer and Tchelepi, 2010; Meyer et al., 2013). It is parametrized in terms of the mean flow velocity, the log-conductivity or -transmissivity correlation length/variance, and provides accurate transport predictions for mildly as well as highly heterogeneous formations.

Our work is structured as follows: In Section 2, we summarize the Gaussian RW model resulting for $\sigma_Y \to 0$ from first-order perturbation theory as outlined in Meyer (2017). The velocity statistics presented in Section 3 were gathered from MC simulations for $\sigma_Y \gg 0$ and enable the quantification and parametrization of deviations from the Gaussian perturbation-theory statistics. In Section 4, the RW model from Section 2 is reformulated in order to account for the non-Gaussian velocity statistics parametrized in Section 3. The accuracy of the resulting refined RW model is assessed in Section 5 and a summary of the present work is provided in Section 6.

2. Random walk from first-order perturbation theory

In this work, we focus on two-dimensional space-stationary formations with multi-Gaussian log-conductivity or -transmissivity distribu-

[2] Plumes that are large enough such that ensemble and spatial averages are interchangeable are referred to as ergodic plumes.

[3] The transmissivity results from a vertical average of the conductivity (Bear, 1972, Section 5.8.1).