Light-Weight Parametrization of Subsurface Spreading for Formations with Small to High Heterogeneity Levels

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Abstract

Reactive subsurface flows are heavily influenced by advective spreading due to flow field heterogeneities. We present a new particle-based model, that relies on stochastic velocity processes similar to CTRW models. Unlike existing approaches, however, we analytically derive our model from first-order perturbation theory and subsequently generalize it for highly heterogeneous formations. The model thus provides a macrodispersion parametrization that is formally consistent with classical results, but also remains accurate for highly heterogeneous formations displaying strong non-Fickian behavior.

Random Walk from Perturbation Theory

Random walk (RW) models have been introduced in subsurface flows as particle-based descriptions of pore-scale dispersion [1] and have been refined and adopted in many applications since [e.g., 2]. Pore-scale RWs operate in physical space and are defined in terms of Langevin or Fokker–Planck equations. More recently, velocity RWs have been proposed to model large-scale spreading induced by flow field heterogeneities [3–6]. The latter result from spatially variable conductivity fields. In this context, continuous time RW (CTRW) models—proposed by Berkowitz et al. [3]—represent an important model category. The CTRW framework was extended and applied by Le Borgne et al. [4], Kang et al. [5], and others for, e.g., fractured formations. In our work, we have recently focused on Langevin-type models that were analytically derived from flow field statistics available from low-order perturbation theory [7]. Unlike previous methods, such an approach induces a model formulation that directly reveals the role of different, potentially space-dependent formation parameters.

More specifically, a Langevin equation for an exemplary velocity process $V(t)$ is given by

$$\mathrm{d}V = D^{(1)}(V)\mathrm{d}t + \sqrt{2D^{(2)}(V)}\mathrm{d}W \text{ with } D^{(m)}(V) \equiv \lim_{\Delta t\to 0} \frac{\langle [V(t+\Delta t) - V(t)]^m | V(t) = V\rangle}{m!\Delta t} \tag{1}$$

and Gaussian Wiener increment $\mathrm{d}W$ having $\langle \mathrm{d}W\rangle = 0$ and $\langle \mathrm{d}W^2\rangle = \mathrm{d}t$. The drift and diffusion coefficients $D^{(1)}(V)$ and $D^{(2)}(V)$ are determined based on Lagrangian velocity transition moments $\langle [V(t+\Delta t) - V(t)]^m | V(t) = V\rangle$. In our present contribution, we have obtained these statistics from first-order perturbation theory [8] for a two-dimensional multi-variate Gaussian geostatistical model for the log-conductivity: In the limit of vanishing heterogeneity, the Lagrangian velocity components $U_1(t)$ and $U_2(t)$ become statistically independent. For example for $U_1(t)$, the velocity transition probability density function (PDF) is then given by

$$f[U_1(t+\Delta t)|U_1(t)] = \frac{1}{\sqrt{2\pi}\sigma_c(t, t+\Delta t)} \exp\left\{ -\frac{[U_1(t+\Delta t) - \mu_c(t, t+\Delta t)]^2}{2\sigma_c(t, t+\Delta t)^2} \right\} \tag{2}$$

with the conditional mean and variance defined as

$$\mu_c(t, t+\Delta t) \equiv \langle U_1\rangle + [U_1(t) - \langle U_1\rangle]\frac{\langle u_1(t)u_1(t+\Delta t)\rangle}{\langle u_1^2\rangle} \text{ and } \sigma_c(t, t+\Delta t)^2 \equiv \langle u_1^2\rangle - \frac{\langle u_1(t)u_1(t+\Delta t)\rangle^2}{\langle u_1^2\rangle},$$

respectively, and $u_1 \equiv U_1 - \langle U_1\rangle$. Based on the velocity covariance $\langle u_i(t)u_j(t')\rangle$ available from first-order perturbation theory [8], the transition moments can be evaluated, leading for example for $U_1(t)$ to

$$\mathrm{d}U_1 = -\frac{8U}{15 l_Y}(U_1 - U)\mathrm{d}t + \sqrt{\frac{2U^3\sigma_Y^2}{5 l_Y}}\mathrm{d}W, \tag{3}$$

with the mean flow velocity U, the log-conductivity variance σ_Y^2, and correlation length l_Y.

Generalization for Highly Heterogeneous Formations

In a subsequent step, an analysis of Lagrangian velocity statistics was performed by means of Monte Carlo (MC) simulation at elevated heterogeneity levels. While for $\sigma_Y^2 \gg 0$, the velocity components U_1 and U_2 become statistically dependent, the angle $\theta \equiv \arctan(U_2/U_1)$ and velocity magnitude remain independent.

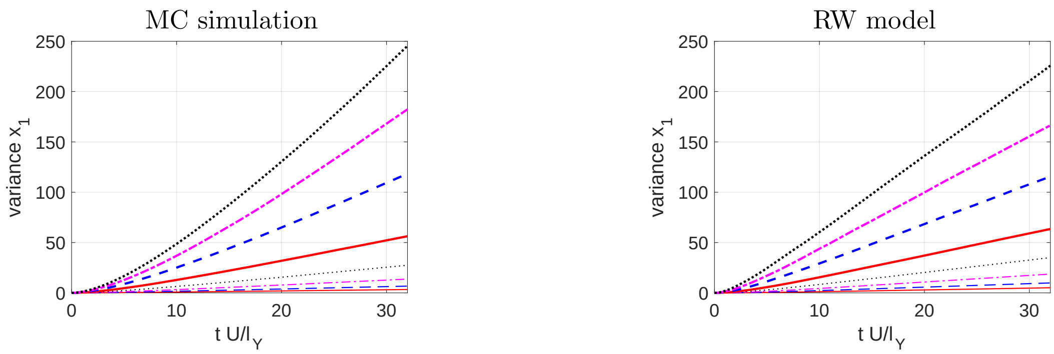

Figure 1: Temporal evolution of the non-dimensional particle position variance in the mean-flow-parallel x_1-direction. Results for (thin solid red) $\sigma_Y^2 = 1/16$, $1/8$, $1/4$, $1/2$, (thick solid red) 1, 2, 3, and (thick dotted black) 4 are provided.

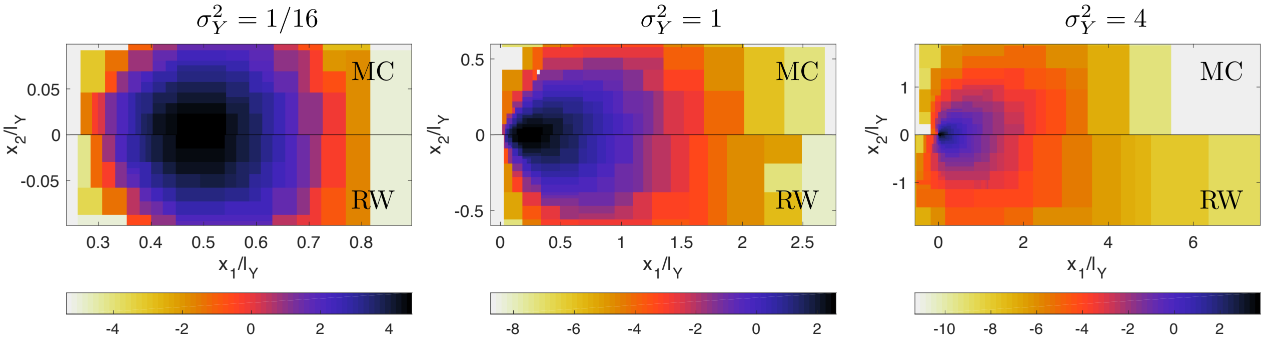

Figure 2: Particle position PDFs for different heterogeneity levels σ_Y^2 resulting at time $t = 0.5 l_Y/U$ from (top halves) MC simulation and (bottom halves) RW model. A logarithmic color scaling is applied.

Moreover, the log velocity-magnitude was found to follow a skew-normal distribution to a good approximation. These observations motivated an analytical reformulation of the U_1–U_2 RW model in terms of processes for θ and the log-velocity $v \equiv \log(|\mathbf{U}|/U)$. The resulting model is directly parametrized in terms of the mean velocity U, the log-conductivity variance σ_Y^2, and correlation length l_Y. It has a compact analytical formulation that is consistent with perturbation theory, but at the same time remains accurate at elevated heterogeneity levels. This is illustrated in Figure 1, where dispersion predictions are assessed against MC-based reference data for a range of heterogeneity levels σ_Y^2. Moreover, in Figure 2, particle position PDFs at an early time—where transport is still far from Gaussian—are inspected for different σ_Y^2.

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