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Impact of local diffusion on macroscopic dispersion in three-dimensional porous media

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While macroscopic longitudinal and transverse dispersion in three-dimensional porous media has been simulated previously mostly under purely advective conditions, the impact of diffusion on macroscopic dispersion in 3D remains an open question. Furthermore, both in 2D and 3D, recurring difficulties have been encountered due to computer limitation or analytical approximation. In this work, we use the Lagrangian velocity covariance function and the temporal derivative of second-order moments to study the influence of diffusion on dispersion in highly heterogeneous 2D and 3D porous media. The first approach characterizes the correlation between the values of Eulerian velocity components sampled by particles undergoing diffusion at two times. The second approach allows the estimation of dispersion coefficients and the analysis of their behaviours as functions of diffusion. These two approaches allowed us to reach new results. The influence of diffusion on dispersion seems to be globally similar between highly heterogeneous 2D and 3D porous media. Diffusion induces a decrease in the dispersion in the direction parallel to the flow direction and an increase in the dispersion in the direction perpendicular to the flow direction. However, the amplification of these two effects with the permeability variance is clearly different between 2D and 3D. For the direction parallel to the flow direction, the amplification is more important in 3D than in 2D. It is reversed in the direction perpendicular to the flow direction.

1. Introduction

Macroscopic dispersion is a key component of solute transport in geological media and is highly influenced by the heterogeneity of geological media ([1], [2]). It is essentially due to its relation to the statistics of flow velocity fields, which has been demonstrated with the first analytical expressions linking velocity and dispersion, given in stratified formations by Matheron et al. [3] and in porous formations by Dagan [4,5], Gelhar et al. [6] and Winter et al. [7].

In his work [8–10], Dagan showed by using the Taylor's work [11] and a Lagrangian framework that the dispersion tensor $D_{t,ij}$ at time t is linked to the auto-covariance tensor C_{ij} of the total displacement $\mathbf{X}_t$:

$$D_{t,ij} = \frac{1}{2}\frac{\mathrm{d}C_{ij}(\mathbf{X}_t)}{\mathrm{d}t} \quad \text{with} \quad C_{ij}(\mathbf{X}_t) = E[\mathbf{X}'_{t,i}\mathbf{X}'_{t,j}] \tag{1}$$

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where $\mathbf{X}_t' = \mathbf{X}_t - E[\mathbf{X}_t]$ is the total displacement fluctuation. Starting its motion at the position $\mathbf{X}_0$ and time t_0, the total displacement of a particle is given by:

$$\mathbf{X}_t(t;\mathbf{X}_0,t_0) = \mathbf{X}(t;\mathbf{X}_0,t_0) + \mathbf{X}_d(t;t_0) \tag{2}$$

The advection displacement $\mathbf{X}$ is related to the flow velocity $\mathbf{u}$:

$$\mathbf{X}(t;\mathbf{X}_0,t_0) = \mathbf{X}_0 + (t-t_0)\mathbf{i} + \int_{t_0}^{t} \mathbf{u}(\mathbf{X}_t)\,\mathrm{d}t' \tag{3}$$

where $\mathbf{i}$ is an unit vector in the x direction. Being a Brownian motion defined by a zero mean and a normal pdf, the local dispersion displacement $\mathbf{X}_\mathrm{d}$ is uncorrelated with $\mathbf{u}$. Then, $C_{ij}(\mathbf{X}_t)$ can be given by:

$$C_{ij}(\mathbf{X}_t) = C_{ij}(\mathbf{X}) + 2(t-t_0)D_{\mathrm{d},ij} \tag{4}$$

where $D_{\mathrm{d},ij}$ is the local dispersion tensor. If diffusion is only considered, $D_{t,ij}$ can be written as:

$$D_{t,ij} = \frac{1}{2}\frac{\mathrm{d}C_{ij}(\mathbf{X})}{\mathrm{d}t} + D_\mathrm{m}\delta_{ij} \quad \text{with} \quad C_{ij}(\mathbf{X}) = \int_{t_0}^{t}\int_{t_0}^{t} C_{ij}(\mathbf{V})\,\mathrm{d}t'\,\mathrm{d}t'' \tag{5}$$

with D_m the diffusion coefficient, δ_{ij} the Kronecker symbol and $C_{ij}(\mathbf{V})$ the Lagrangian auto-covariance tensor computed from the velocity sampled by the particles undergoing diffusion. The previous equation can be re-written as:

$$D_{t,ij} = \frac{1}{2}\int_{t_0}^{t} C_{ij}(\mathbf{V})\,\mathrm{d}t' + D_\mathrm{m}\delta_{ij} \tag{6}$$

This equation clearly shows the role played by diffusion. In addition to participating in the spreading of particles, diffusion modifies the sampling of the Eulerian velocity by the particles. Then, the analysis of the influence of diffusion on dispersion depends on the estimation of the Lagrangian auto-covariance tensor. Following the analytical approach and under simplification assumptions, this auto-covariance tensor can be expressed with different methods such as the Corsin's conjecture ([9], [12], [13]) and the perturbation theory ([10], [14], [15]). However, the analytical solution only gives valid results for weakly heterogeneous permeability fields ([16]). While the numerical approach does not require an approximation of the velocity auto-covariance tensor except in some cases ([17]), it is still confronted with convergence issue at higher values of heterogeneity, especially in 3D, and the macroscopic dispersion coefficients do not always reach an asymptotic value as described in a Fickian regime ([18], [19], [20]). While in these works, the macroscopic dispersion coefficients are computed through the particle positions and the second-order moments, equation (6) enables the macroscopic dispersion coefficients to be calculated from the Lagrangian velocity covariance. This method has been used in Salandin et al. [21] and later Gotovac et al. [22] with Monte Carlo simulations where particles are tracked but are limited to pure advection cases in isotropic 2D heterogeneous porous media.

In this work, we compute the Lagrangian velocity covariance functions for pure advection and diffusion cases in isotropic highly heterogeneous 2D and 3D porous media. To obtain a well-defined covariance function, we use high performance computing with the numerical model PARADIS, PARAllel DISpersion, available in the software platform H2OLAB (http://h2olab.inria.fr/) to compute the particles trajectories. PARADIS performs large-scale and finely resolved Monte Carlo simulations for estimating the trajectory of inert particles in heterogeneous porous media characterized by an exponentially correlated log-normal isotropic permeability fields ([23,24], [25,20]). These previous works focus on advective and diffusive conditions in 2D and purely advective in 3D. Furthermore, the macroscopic coefficients are computed through the temporal derivation of particle cloud second-order moments. This work introduces the effect of diffusive condition and a numerical analysis of Lagrangian velocity covariance functions, which allows the identification of the impact of local diffusion on dispersion in 2D and 3D.

2. Covariance function computing

The covariance function C_{ii} of the component V_i of the Lagrangian velocity $\mathbf{V}$ can be estimated as follows:

$$C_{ii}(\mathbf{V}) = \sigma_{V_i}^2 - \gamma_{V_i}(h) \tag{7}$$

where $\sigma_{V_i}^2$ and γ_{V_i} are the variance and variogram of V_i respectively; h represents the time step between two times. To compute γ_{V_i}, the stochastic variable V_i has to respect two properties: