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Determination of the diffusivity, dispersion, skewness and kurtosis in heterogeneous porous flow. Part II: Lattice Boltzmann schemes with implicit interface

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A B S T R A C T

A simple local two-relaxation-time Lattice Boltzmann numerical formulation (TRT-EMM) of the extended method of moments (EMM) is proposed for analysis of the spatial and temporal Taylor dispersion in *d*-dimensional streamwise-periodic stationary mesoscopic velocity field resolved in a piecewise-continuous porous media. The method provides an effective diffusivity, dispersion, skewness and kurtosis of the mean concentration profile and residence time distribution. The TRT-EMM solves a chain of steady-state heterogeneous advection–diffusion equations with the pre-computed space-variable mass-source and automatically undergoes diffusion-flux jump on the abrupt-porosity streamwise-normal interface. The temporal and spatial systems of moments are computed within the same run; the symmetric dispersion tensor can be restored from independent computations performed for each periodic mean-velocity axis; the numerical algorithm recursively extends for any order moment.

We derive an exact form of the bulk equation and implicit closure relations, construct symbolic TRT-EMM solutions and determine specific relation between the equilibrium and the collision degrees of freedom viewing an exact parameterization by the physical non-dimensional numbers in two alternate situations: "parallel" fracture/matrix flow and "perpendicular" Darcy flow through porous blocks in "series". Two-dimensional simulations in linear Brinkman flow around solid and through porous obstacles validate the method in comparison with the two heterogeneous direct LBM-ADE schemes with different anti-numerical-diffusion treatment which are proposed and examined in parallel. On the coarse grid, accuracy of the three moments is essentially determined by the free-tunable collision rate in all schemes, and especially TRT-EMM. However, operated within a single periodic cell, the TRT-EMM is many orders of magnitude faster than the direct solvers, numerical-diffusion free, more robust and much more capable for accuracy improving, high Péclet range and free-parameter influence reduction with the mesh refinement. The method is an efficient predicting tool for the Taylor dispersion, asymmetry and peakedness; moreover, it allows for an optimal analysis between the mutual effect of the flow regime, Péclet number, porosity, permeability and obstruction geometry.

1. Introduction

Understanding of the structure and velocity influence on the mass transport, prediction and optimization of the Taylor and environmental dispersion, elongated tails of the averaged (upscaled) solute distributions and their time-rate, the residence-time distribution RTD, is a task required in many engineering fields, such as chemical, polymer, petrol, agricultural, ecological risk assessment and restoration, wastewater treatment. We propose a simple numerical method for prediction of the first four moments of the solute distribution from the steady-state velocity field established in the streamwise-periodic representative unit cell. Especially, we keep in mind a direct application in X-ray microtomography images of the double porosity media, like the carbonates, where the proposed method allows for the rock identification and classification with respect to the dispersion and non-Gaussian properties of the breakthrough curves.

Within the dispersion theory, established in fundamental works by Taylor (1953), Aris (1956) and Brenner (1980), the Gaussian description applies to upscaled distributions with the longitudinal Taylor dispersion correction (Aris, 1956; Taylor, 1953) to molecular diffusion coefficient [hereafter, D_T and $\mathcal{D}_0$, respectively] or, more generally, full dispersion tensor (Brenner, 1980) due to the multi-dimensional gradients in velocity field. The classical approach is focused on the *spatial* solute evolution after an instantaneous point release, when the distribution moments are computed via the spatial integration. The RTD introduced by Danckwerts (1953) is commonly monitored in the outlet of the chemical device (Cozewith and Squire, 2000), vegetation zone for pollutant

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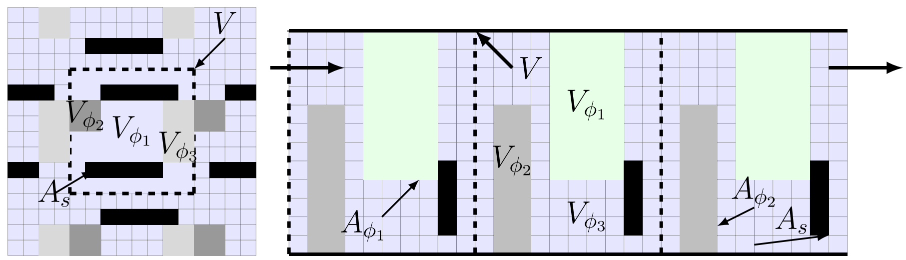

Fig. 1. Sketches for the heterogeneous obstacles or a composite material filled with the porous media, and a porous/solid/vegetation arrangement for dispersion reduction within an unit periodic cell V.

remediation (Werner and Kadlec, 2000) or micro-channel (Cantu-Perez et al., 2008), and it can be characterized through the *temporal* moments integrated in time (Vikhansky, 2011). The Taylor regime is respectively characterized by a time and space linear growing of the variance, like $\sigma^2 = 2(\mathcal{D}_0 + D_T)t$ at a dimensionless time $t' = t\mathcal{U}_0/\mathcal{L} \geq\approx$ Pe, or $\sigma^2 = 2\mathcal{U}_0^{-3}(\mathcal{D}_0 + D_T)x$ at a dimensionless distance $x' = x/\mathcal{L} \geq\approx$ Pe [hereafter, Pe $= \frac{\mathcal{U}_0\mathcal{L}}{\mathcal{D}_0}$ is the characteristic Péclet number]. However, many natural systems exhibit asymmetry, peakedness and heavy tails, a long time or distance after release. So far, the Taylor dispersion theory fails to explain the non-Fickian behavior of the molecular propagators in heterogeneous porous beds (Berkowitz et al., 2008; Bijeljic et al., 2011), successfully reproduced by the numerical simulations in double porosity carbonates (Bijeljic et al., 2013; Yang et al., 2013). Recent studies suggest that considering the vegetation as a porous zone offers a promising prediction of the pollutant retention RTD observed in the experimental vegetated channels and pond systems (see review Golzar, 2015). The open question lies in the optimal design (Su et al., 2009) of the remediation zones through their permeability (resistance), porosity and geometric obstruction. The high-order moments quantify the deviations from the normal distribution: the skewness (Sk, third-order moment) and kurtosis (Ku, fourth-order moment) are responsible for the asymmetry and peakedness, respectively. Let us assume that a continuous velocity field $\vec{u}_\phi(\vec{r})$ is resolved in a heterogeneous piece-wise-continuous porosity distribution $\phi(\vec{r})$ [we keep in mind a sketch in Fig. 1]. A complete evolution history needs to solve the d-dimensional advection–diffusion equation (ADE) for the continuous concentration $C(\vec{r}, t)$:

$$\partial_t(\phi C) + \nabla \cdot (\vec{u}_\phi C) = \nabla \cdot (\phi \mathbf{D}^{(0)} \cdot \nabla C),\ \nabla \cdot \vec{u}_\phi = 0,\ \vec{r} \in V_\phi. \quad (1)$$

The Taylor dispersion coefficient D_T is the same in the two systems of moments: spatial, $\langle\phi\rangle^{-1}\langle x^n C\phi\rangle$ and temporal, $\int_{-\infty}^{\infty} t^n P(x,t)dt$, $P(x,t) = \partial_t\langle C(x,t)\rangle$ [the brackets denote averaging over the fluid part of a single periodic cell, $\{V_\phi\} \in V$ in Fig. 1]. However, the higher-order moments differ in the two systems; their computation requires specific initial/boundary set-up with the direct ADE solvers of Eq. (1) and leads to a tedious numerical task combining the highly discontinuous diffusion coefficients in complex interface/boundary geometry with the high Péclet numbers. In a periodic arrangement, the solute evolution is run through a long series of duplicated cells [V in Fig. 1]; since their number increases with Pe, the computational time to the Taylor regime grows as Pe^2, at least.

The Brenner's B-method of moments (Brenner, 1980) circumvents the problem: it restores the symmetric dispersion tensor $\mathbf{D}[d \times d] = \frac{\mathcal{D}_0}{V_\phi}\langle\nabla(\mathbf{B} - \vec{r})^t\nabla(\mathbf{B} - \vec{r})\rangle$ independently solving d steady-state advection–diffusion equations for space-periodic vector-variable $\mathbf{B}[d]$ *inside a single cell*. The finite-difference scheme (Salles et al., 1993) validated the B-method in microscopic three-dimensional Stokes flow through the regular, fractal, random and reconstructed porous media. A similar dispersion boundary-value problem was recently parameterized (Valdés-Parada et al., 2016) with the Reynolds number in slow inertial flow through an uniform soil porosity. The *extended method of moments* (EMM) extends the dispersion procedure to heterogeneous soil and any-order spatial or temporal moments. Originated from the ideas (Vikhansky, 2008) and substantial developments (Vikhansky and Ginzburg, 2014), the EMM is elaborated (Ginzburg and Vikhansky, 2018) in the form of the recursive algorithm for prediction of (i) effective diffusion (structure) coefficient, (ii) Taylor dispersion dyadic, and (iii) longitudinal coefficients of the high-order moments. Differently from the Brenner's averaging of the Brownian particles moments or the volume-averaging approach (Valdés-Parada et al., 2016), the EMM searches for the solution of Eq. (1) in the form of a product of the low frequency, slow monochromatic wave and a streamwise-periodic (say, along the x-axis) oscillating scalar field $B(\omega, \gamma; \vec{r})$:

$$C(\vec{r}, t) = \frac{1}{2\pi} B(\omega, \gamma; \vec{r}) \exp[i(\gamma x - \omega t)]. \quad (2)$$

A simultaneous perturbative expansion is performed either for $B(\omega(\gamma), \vec{r})$ and temporal frequency $\omega(\gamma)$, or for $B(\gamma(\omega), \vec{r})$ and wavenumber $\gamma(\omega)$; the mathematical algorithms based upon are referred to as "ω-form" and "γ-form", respectively:

$$\text{"}\omega\text{-form"}: \ B(\omega, \gamma; \vec{r}) = \sum_{n=0}^{\infty} B_n(\vec{r})(i\gamma)^n,\ \omega(\gamma) = -i\sum_{n=1}^{\infty}\omega_n(i\gamma)^n, \quad (3a)$$

$$\text{"}\gamma\text{-form"}: \ B(\omega, \gamma; \vec{r}) = \sum_{n=0}^{\infty} B_n(\vec{r})(i\omega)^n,\ \gamma(\omega) = -i\sum_{n=1}^{\infty}\gamma_n(i\omega)^n. \quad (3b)$$

In both formulations, the (B-field) variable $B_n(\vec{r})$ solves a chain of steady-state ADE with the recursively-built mass-sources. The two sets $\{\omega_n\}$ and $\{\gamma_n\}$ are determined explicitly from the global mass conservation solvability condition; they sequentially determine the dispersion, skewness and kurtosis ($n = 2, 3, 4$, respectively) in spatial and temporal, respectively, system of moments; the solution procedure straight forwardly extends to any higher-order moment. Since the coefficients of the two expansions are inter-related through simple algebraic formulae, the two sets of moments become determined within the same solution path. In a streamwise-uniform duct flow, the EMM moments correspond (Ginzburg and Vikhansky, 2018) to the (upscaled) mean-concentration solution obeying the high-order PDE (Mercer and Roberts, 1990; Ngo-Cong et al., 2015) without need to resorting for its solving.

The EMM allows for the symbolic moments prediction in continuous parameter space. So far, the Taylor dispersion, skewness and kurtosis were exemplified (Ginzburg and Vikhansky, 2018; Vikhansky and Ginzburg, 2014) in (i) parabolic (Poiseuille) profile in a channel and cylindrical capillary, (ii) non-Newtonian power-law flow in a capillary, (iii) shallow profile through different cross-section shapes, (iv) Darcy–Brinkman flow in stratified fracture/matrix layers and (v), a "perpendicular" Darcy flow through porous blocks. These solutions allow to estimate the role of the porosity contrast and geometry aspect in the first four moments, also providing their asymptotic Pe-scaling. The reference EMM solutions give the valuable benchmarks for direct solvers of Eq. (1) and numerical EMM formulations. Furthermore, applying the EMM decomposition to the effective, fourth-order-accurate mass-conservation equation of a numerical scheme, the truncation interference with the physical moments may become quantified quasi-exactly