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Simulation of solute dispersion in particle packs by the volume averaging method

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ABSTRACT

The ability to predict solute dispersion behavior in homogeneous random particle packs by the volume averaging method is evaluated. Unit cells with periodic boundaries and random pore connectivity are numerically constructed. The asymptotic longitudinal and transverse dispersion coefficients are predicted by the volume averaging method in terms of these unit cells. The Peclet number is in the range of 0–1000. The Reynolds number is less than 1. Dispersion coefficients of eighteen unit cells with different sizes and pore geometries are compared. It is found that a significant scatter of dispersion coefficients exists when the size of the unit cell is small. The scatter decreases with increasing size of the unit cell. The predicted dispersion coefficients are compared with correlations obtained according to experimental and simulation results for homogeneous random particle packs and reasonable agreements are observed when the size of the unit cell is suitable.

1. Introduction

Solute transport in porous media is an important issue in fields of chemical engineering, environment, analytical chemistry. Understanding the phenomenon is important for many applications, such as solute separation in packed beds and chromatography columns, contaminant migration in soil. A solute band in the moving fluid will move with the fluid, and simutaneously, the band will broaden. The band broadening phenomenon is usually called solute dispersion.

The dispersion phenomenon in porous media is usually characterized by the longitudinal (along the mean flow direction) and transverse (perpendicular to the mean flow direction) dispersion coefficients. Accurate results of dispersion coefficients are important for the design of adsorption separation devices or the control of process operation parameters for many process industries. Many experimental data and correlations are available in the literature (Delgado, 2006; Bons et al., 2013; Scheven et al., 2007; Scheven, 2013; Scheven et al., 2014), but significant scatter exists (Delgado, 2006). The scatter may be caused by the difference of the pore geometry in different experiments. The pore geometry of particle packs depends on many factors, such as the packing method, wall confinement, particle shape and size distributions. It is difficult or impossible to make two sets of particle packs the same. A slight inhomogeneity of the pore geometry may introduce a significant flow heterogeneity and thus may result in a significant dispersion coefficient deviation. Recently, consistent results for different random particle packs were reported by nuclear magnetic resonance (NMR) based experiments (Scheven et al., 2007; Scheven, 2013; Scheven et al., 2014). The unavoidable macroscopic flow heterogeneities were separated by their data analysis. They reported that the flow profile at the pore level did not appear to have pronounced effects on the longitudinal dispersion coefficient in the mechanically mixed regime (the Peclet number ranging from 10 to 450). Simulation of solute dispersion in spatially periodic particle packs by the Lattice-Boltzmann method (LBM) and particle tracking method (Scheven et al., 2014) confirm the experimental results. These accurate experimental data make it possible to verify the accuracy of simulation approaches.

Many researchers (Scheven et al., 2014; Maier et al., 2000; Freund et al., 2005; Koku et al., 2012; Hlushkou et al., 2013) simulated the flow and mass transport behaviors in porous media by the combination of LBM and the particle tracking method. In recent years, the conventional computational fluid dynamic (CFD) method was also used to simulate the flow and mass transport problem in porous media (Augier et al., 2008; Jafari et al., 2008; Augier et al., 2010; Parthasarathy et al., 2013; Loh and Vasudevan, 2013; Jourak et al., 2013; Baker et al., 2014). Both methods show their ability to achieve reasonable simulation results. The transient mass transport behavior was simulated by these methods (Scheven et al., 2014;

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Nomenclature

A_p	Surface area of pores in a unit cell, m^2
C	Solute concentration, mol/m^3
$<C>$	Solute concentration averaged in pores of a unit cell, mol/m^3
d_p	Particle diameter after contraction, m
d_{p0}	Particle diameter before contraction, m
D_m	Solute molecular diffusion coefficient, m^2/s
D_L	Longitudinal dispersion coefficient, m^2/s
D_{Ty}, D_{Tz}	Transverse dispersion coefficient along the direction of y-axis and z-axis, respectively, m^2/s
f_L	Closure variable corresponding to longitudinal dispersion coefficient, m
f_{Ty}, f_{Tz}	Closure variables corresponding to transverse dispersion coefficient, m
l_g	Gap size between neighbour blocks, m
l_{bx}, l_{by}, l_{bz}	Lengths of the rectangular block along the three independent axies, m
l_x, l_y, l_z	Lengths of the unit cell along the three independent axies, m
n_L, n_{Ty}, n_{Tz}	Components of the normal unit vector at pore surface along the x-axis, y-axis, z-axis, respectively
p	Fluid static pressure, Pa
Pe	Peclet number
u, v, w	Fluid velocity component along the x-axis, y-axis and z-axis, respectively, m/s
u_i	Mean flow velocity along the main flow direction in pores of a unit cell, m/s
$\mathbf{v}$	Fluid velocity vector, m/s
V_m	Volume of the liquid region in a unit cell, m^3
μ	Fluid viscosity, Pa.s

Maier et al., 2000; Freund et al., 2005; Koku et al., 2012; Hlushkou et al., 2013; Augier et al., 2008; Jafari et al., 2008; Augier et al., 2010; Parthasarathy et al., 2013; Loh and Vasudevan, 2013; Jourak et al., 2013; Baker et al., 2014). The volume averaging method (VAM) is an alternative method for solving the mass transport problem in porous media (Carbonell and Whitaker, 1983; Quintard and Whitaker, 1993; Buyuktas and Wallender, 2004; Wood, 2007; Plumb and Whitaker, 1988; Cherblanc et al., 2007; Quintard et al., 2006; Coutelieris et al., 2006; Vales-Parada et al., 2011; Yan et al., 2010; Yan et al., 2015). Being different from above two methods, VAM is used to calculate the asymptotic dispersion coefficient by solving a steady state closure problem instead of the transient solute transport problem. In addition, a unit cell with periodic boundary geometry must be constructed to solve the closure problem. Thus, the dispersion coefficient calculated by VAM is actually for spatially periodic porous media.

The solute dispersion coefficients for random particle packs were successfully predicted by LBM and the particle tracking method with the aid of spatially periodic particle packs (Scheven et al., 2014), which indicates the feasibility of using spatially periodic particle packs to predict dispersion coefficients of random particle packs. However, no successful prediction has been reported when VAM combined with spatially periodic particle packs are used. Dispersion coefficients calculated by VAM for the two dimensional spatially periodic particle packs (Buyuktas and Wallender, 2004) and three dimensional ordered particle packs (Wood, 2007) deviated obviously from experimental data for random particle packs. Up to now, it is difficult to judge whether VAM can be used confidently to predict the dispersion for flow through homogeneous random particle packs.

A reliable numerical approach to predict the solute transport behavior in random particle packs is important in that it can be complement with experiments to guide new design or scale-up of industrial setups. The aim of this paper is to compare the dispersion behaviors for flow through the random particle packs and the spatially periodic particle packs with local random pore connectivity, so that we can evaluate the ability of VAM in predicting the dispersion for flow through homogeneous random particle packs.

2. Dispersion prediction method

2.1. Spatially periodic particle packs and the physical problem

The random particle pack is constructed by the following approach. Firstly, 4730 spherical particles with the same diameter d_{p0} are packed in a square column ($16d_{p0} \times 16d_{p0} \times 20d_{p0}$) by the discrete element method (Cundall and Strack, 1979; Zhu et al., 2007). Implementation of the method is validated in previous study (Yang et al., 2016). Random close packing is realized with the porosity of 0.378. Secondly, particles are contracted to form floating particles with a diameter of d_p. This contraction is done for the ease of generating mesh for numerical simulation (Augier et al., 2010). The effect of particle contraction on the dispersion coefficient is discussed in a later section.

The process to construct the spatially periodic particle pack is schematically described in Fig. 1a. Firstly, a rectangular block (the size of the block (l_{bx}, l_{by}, l_{bz}) is shown in Table 1) in the random particle pack is chosen. Particles intersecting with the rectangular block are trimed to reserve the region inside the rectangular block, as shown in Fig. 1b. Secondly, the block is copied and arranged in an ordered configuration to form a new particle pack, as shown in Fig. 1a. The particle block as shown in Fig. 1(b) is not a spatially periodic porous media, while VAM only can be used to predict the solute dispersion behavior for spatially periodic porous media. We solve this problem by arranging a gap (shown in Fig. 1(a)) between neighbour particle blocks so that the new particle pack is periodic globally. Although the new particle pack can be considered as spatially periodic globally, the local random pore connectivity inside a particle block is similar to that of random particle packs. A unit cell of the spatially periodic particle pack is schemetically shown in Fig. 1a. The effect of the gap on the dispersion coefficient is discussed in a later section.

Our computational domain is the fluid region in a unit cell. Sizes of the unit cell and porosity of spatially periodic particle packs are shown in Table 1. l_x, l_y and l_z are the lengths of the unit cell along three independent axies. x-axis is the main flow direction.

Liquid filled in pores of particle packs and was driven by pressure. Solute dissolved in the liquid disperses in the pores among particles. No surface reaction or adsorption occurs on the pore surfaces. The dispersion behavior is time-dependent but the asymptotic behavior exists when the porous media region is large, which is the case of most chemical engineering applications. In this paper, we focus on the asymptotic dispersion behavior. The fluid Schmidt number is 1000, and the Peclet number ranges from 0.1 to 1000. Accordingly, the Reynolds number is less than 1, implying a negligible inertial effect. Under this situation, the difference of the velocity solutions obtained by solving the Stokes equation and the Navier-Stokes equation is negligible. So, we solve the Stokes equation.

2.2. The volume averaging method

The velocity vector for liquid flowing through particle packs is calculated by solving the Stokes equation:

$$\nabla p = \mu \nabla^2 \mathbf{v} \tag{1}$$