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Pore-scale simulation and statistical investigation of velocity and drag force distribution of flow through randomly-packed porous media under low and intermediate Reynolds numbers

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ABSTRACT

Fluid flow through packed porous media and fluid–particle interactions are of importance in various industrial and natural processes. However, the lack of knowledge about the velocity field in the pore space and distribution of drag force on individual particles has been a source of uncertainties in modeling these processes. Therefore, an improved understanding of the velocity field and fluid–particle interactions is a fundamental step for better understanding of these systems. In this article, the pore-scale velocity field and fluid–solid interaction from a single particle to randomly-packed mono-sized porous media are investigated using a 3D GPU-based parallel Lattice Boltzmann model. The packed porous media are generated by means of discrete element method and have a wide range of porosity values. The developed model is first validated by experimental results of fluid flow around single and two interactive particles; the validated model is then used to conduct statistical analysis of velocity in the pore space and drag force on individual particles. The results suggest that the velocity field in porous media can be divided into four zones, namely: zero-velocity zone, low-velocity zone, high-velocity zone, and recirculation zone. Moreover, the probability density distribution of velocity is highly dependent on Reynolds number and porosity and can be bi-modal, depending on a combination of Reynolds number and porosity. The probability density distribution of the drag force always shows a single peak at the mean value with a skewness to the right. Finally, a simpler and more accurate correlation for the mean drag force over a wide range of Reynolds number and porosity is proposed based on the numerical results. The accuracy and reliability of several empirical equations, including the one proposed in this study, for the mean drag force are compared through a statistical analysis.

1. Introduction

Fluid flow through packed porous media is of importance to various geological [27], petroleum [39], and industrial processes [35]. Understanding the velocity field at pore scale and relative motion between fluid and solid particles is important because the non-uniform velocity field leads to the formation of non-uniform force field and fluid–particle interactions in a packed porous media. Knowledge of the velocity field is also a key to understanding the zero-, low-, and high-velocity zones where mass convection and diffusion are likely to occur.

Over the past decades, fluid flow through packed porous media has been studied using experimental and numerical approaches [21,38,51]. Although experimental techniques such as laser-Doppler anemometry [46], radioactive particle [7] and the magnetic resonance imaging tracking [40] are useful, they are difficult and time consuming. It is often infeasible to collect measurement data of the drag force on individual particles in porous media. With increased computational capability, numerical simulation of pore-scale fluid flow in porous media has become feasible. Among different numerical methods, the lattice Boltzmann (LB) method is a promising one. The LB method is based on statistical molecular description of a fluid and is capable of solving complex physical phenomena directly based on the statistical interaction between molecules. A main advantage of the LB method is its capability in accommodating irregular interfaces in inhomogeneous flow, such as those in porous media. Maier et al. [30] used the LB method to study the spatial velocity distribution in a packed column of glass beads. They reported that the normalized velocity distributions are approximately the same for different packed beds with porosities in the range of 0.52–0.65 and particle Reynolds (Re) number in the range of 0.5–29. Tobis [41] used unit-cell method to investigate the turbulent flow in a packed bed. Magnico [29] conducted unit-cell

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simulations and investigated flow structures on mass transfer. Recently, Rong et al. [36] used LB method to investigate the effect of porosity (ε) and *Re* number on the velocity distribution in porous media for porosities in the range of about 0.36–0.77.

Estimate of the drag forces from fluid–solid interaction is important in modeling packed porous media and fluidized bed. For example, the drag force terms are needed in coupling fluid motion and solid motions in fluidized bed and seepage problems (e.g., [13]). The exact solution is available only for the case of porosity near one and *Re* number near zero (i.e., Stokes law). Historically, researchers have proposed equations based on empirical data of either the pressure drop or terminal velocities of porous media to estimate the mean drag force for a wide range of *Re* numbers, porosities, and particle diameters. For example, the Ergun [14] correlation is derived from pressure drop measurements and the Wen and Yu [44] correlation is derived from terminal velocity. Recently, researchers have also utilized LB simulation results to develop equations for the mean drag force. For example, Hill et al. [19,20] were the first to develop equations valid for different ranges of *Re* numbers and porosities, and Van der Hoef et al. [43] extended the work of Hill et al. [19,20] and proposed new mean drag force equation based on the Carman–Kozeny equation. Beetstra et al. [2] conducted LB simulations with up to 32 particles and investigated the effect of inter-particle distance on the mean drag force. Yin and Sundaresan [47] proposed a correlation for laminar flow in fixed particle configuration. Zhang et al. [48] used 2D LB simulations to investigate the effect of particle cluster in the domain on the mean drag force. Recently, Rong et al. [36] modified drag force correlation proposed by Di Felice [12]. However, the accuracy and reliability of current empirical equations for drag force have not been evaluated and compared over a wide range of porosities and *Re* numbers.

This paper presents a statistical investigation on the velocity and drag force distributions of fluid flow through packed porous media over a wide range of porosities and *Re* numbers using the LB method, which has not been comprehensively studied before. A GPU-based 3D LB model is developed to simulate a domain with up to 9800 solid particles, which is more realistic than the limited number of particles considered by previous LB models. For example, Rong et al. [36] considered 324–805 solid particles depending on the porosity, which is the most number of particles considered thus far in LB simulations and not sufficient for statistical investigation. Based on the LB simulation results in this study, a new equation for the mean drag force is developed and compared with other equations available in the literature. In the following sections, the LB method is first introduced, followed by the development and validation of the LB model. The simulated pore-scale velocity and drag force distributions for fluid flow through monosized randomly-packed porous media are analyzed and statistically investigated for a wide range of porosities and *Re* numbers.

2. Numerical method

2.1. Lattice Boltzmann method

The LB method is a particle-based meso-scale numerical method and has been used to solve the Navier–Stokes equations. Its strength in comparison with conventional CFD methods lies in its ability to efficiently interact with complex physical phenomena and/or irregular geometry such as those in fluid flow through porous media. The LB method is also suitable for parallelization in high performance computing. In this study, a GPU-based 3D nineteen discrete velocities (D3Q19) LB method [11,26] is used for simulating fluid flow in packed porous media. The LB formulations are briefly presented below. The LB equations can be written in the following form:

$$\mathrm{f}_i(\boldsymbol{X}+\boldsymbol{e}_i\delta_t, t+\delta_t) - \mathrm{f}_i(\boldsymbol{X}, t) = \Omega \quad i = 0, 19 \tag{1}$$

where $\mathrm{f}_i(\boldsymbol{X}, t)$ is the density distribution function for the ith velocity direction at position $\boldsymbol{X}$ and time t, $\boldsymbol{e}_i$ is the discrete velocity, δ_t is the time increment, and Ω is the collision operator. Evolution of the fluid in the domain by LB method during each time step has two main phases: collision and streaming. In collision, particles collide and scatter according to a collision operator: the right-hand side of Eq. (1); in streaming, particles move to the nearest neighbor nodes according to their velocities. In doing so, the streaming phase explicitly propagates the updated distribution function at each node to its neighbors $\boldsymbol{X}+\boldsymbol{e}_i\delta_t$: left hand side of Eq. (1).

In this study, the multiple-relaxation time (MRT) scheme [11,32] is adopted as the collision operator because the MRT scheme is advantageous in enhancing numerical stability and viscosity-independent boundary conditions [33,38] over the well-known BGK approximation [9]. With the MRT scheme, the collision operator is given by:

$$\Omega = -\left(M^{-1}SM\right)\left(f_i - f_i^{eq}\right) + \phi_i, \tag{2}$$

where M is a transformation matrix [11,26] and S is a diagonal relaxation matrix defined by:

$$S = diag(s_\nu,\ s_e,\ s_\varepsilon,\ s_\nu,\ s_q,\ s_\nu,\ s_q,\ s_\nu,\ s_q,\ s_\nu,\ s_\pi,\ s_\nu,\ s_\pi,\ s_\nu,\ s_\nu,\ s_\nu,\ s_m,\ s_m,\ s_m), \tag{3}$$

where the element s_i is the relaxation rate associated with each f_i. The relaxation parameter s_ν which determines the viscosity υ is:

$$\upsilon = \frac{1}{3}\left(\frac{1}{s_\nu} - \frac{1}{2}\right) \tag{4}$$

There are five other adjustable relaxation parameters: s_e, s_ε, s_π, s_m and s_q, which are set to be identical values to preserve symmetry on the chosen lattice as follows [33]:

$$s_e = s_\varepsilon = s_\pi = s_m = s_q = 8\frac{2-s_\nu}{8-s_\nu} \tag{5}$$

In Eq. (1) f_i^{eq} is the equilibrium distribution function of f_i and a popular choice is [45]:

$$f_i^{eq} = \rho w_i\left[1 + \frac{3}{c^2}\boldsymbol{e}_i.\boldsymbol{u} + \frac{9}{2c^4}(\boldsymbol{e}_i.\boldsymbol{u})^2 - \frac{3}{2c^2}\boldsymbol{u}^2\right], \tag{6}$$

where ρ and $\boldsymbol{u}$ are fluid density and velocity respectively ($\rho = \sum_i \mathrm{f}_i$, $\boldsymbol{u} = \sum_i \boldsymbol{e}_i\mathrm{f}_i/\rho$) and w_i is the weighting factor with $w_0 = 12/36$, $w_{1-6} = 2/36$ and $w_{7-18} = 1/36$. The additional term ϕ_i in Eq. (2) is given by $\phi_i = w_i e_i G$ where G is body force.

In order to obtain acceptable results from LB simulations, especially for fluid flow in packed porous media, several items should be carefully considered. First, a constraint to the parameter selection is the lattice speed C, defined as $C = \delta h/\delta t$ where δh is lattice spacing. Lattice speed must be sufficiently larger than the maximum fluid velocity $\boldsymbol{u}_{max}$ in the simulation domain to ensure sufficient solution accuracy and incompressibility of the fluid. This is controlled by the computational Mach number ($Ma = |\boldsymbol{u}_{max}|/C$). Theoretically, it is required that $Ma \ll 1$; in practice, Ma should be smaller than 0.1.

Second, each of the individual particles in the porous domain should be made of enough lattices so that lattice-independent results can be obtained. In order to identify the optimal lattice resolution for this study, the total viscous drag force of a simple cubic array of spheres in the middle of a flow field with a constant pressure gradient is simulated and compared with analytical solutions. Hasimoto [17] proposed the following equation for the total drag force on a viscous flow passing a simple cubic array of spheres:

$$\frac{3\pi\rho\nu dU}{F_{total}} = 2 - 1.76(1-\varepsilon)^{\frac{1}{3}} - \varepsilon - 1.559(1-\varepsilon)^2, \tag{7}$$