Advanced Powder Technology xxx (2017) xxx–xxx

Contents lists available at ScienceDirect

Advanced Powder Technology

journal homepage: www.elsevier.com/locate/apt

Original Research Paper

Lattice Boltzmann simulation of flow past a non-spherical particle

Yanjun Guan [a,b], Rodrigo Guadarrama-Lara [b], Xiaodong Jia [b], Kai Zhang [a,*], Dongsheng Wen [b,c,*]

[a] Beijing Key Laboratory of Emission Surveillance and Control for Thermal Power Generation, North China Electric Power University, Beijing 102206, China
[b] School of Chemical and Process Engineering, University of Leeds, Leeds LS2 9JT, UK
[c] Laboratory of Fundamental Science on Ergonomics and Environmental Control, School of Aeronautic Science and Engineering, Beihang University, Beijing 100191, China

A R T I C L E I N F O

Article history:
Received 8 November 2016
Received in revised form 2 February 2017
Accepted 16 March 2017
Available online xxxx

Keywords:
Lattice Boltzmann method
Spherical particle
Non-spherical particle
Drag coefficient
Low-to-high Reynolds number

A B S T R A C T

Lattice Boltzmann method was used to predict the fluid-particle interaction for arbitrary shaped particles. In order to validate the reliability of the present approach, simulation of flow past a single stationary spherical, cylindrical or cubic particle is conducted in a wide range of Reynolds number ($0.1 < Re_p < 3000$). The results indicate that the drag coefficient is closely related to the particle shape, especially at high Reynolds numbers. The voxel resolution of spherical particle plays a key role in accurately predicting the drag coefficient at high Reynolds numbers. For non-spherical particles, the drag coefficient is more influenced by the particle morphology at moderate or high Reynolds numbers than at low ones. The inclination angle has an important impact on the pressure drag force due to the change of projected area. The simulated drag coefficient agrees well with the experimental data or empirical correlation for both spherical and non-spherical particles.

1. Introduction

Gas-solids flow systems are widely encountered in chemical and process industries. The comprehensive knowledge of the gas-solids flow characteristics is essential for the scale-up, design and optimization of chemical reactor and improvement of system efficiency [1,2]. Computational Fluid Dynamics (CFD) has been regarded as an effective alternative approach for understanding the complex physics of gas-particle flow, which presents a big challenge experimentally due to the limitation of measuring techniques. Accurate description of the drag force between the gas and particle phase is one of the key issues for CFD modeling of gas-solids flow [3–5]. Up to now, most of the drag models are developed from spherical particles, such as the Wen-Yu model [6], Syamlal-O'Brien model [7], Gidaspow model [8] and Energy Minimization Multi-Scale model [9]. However, a noteworthy fact is that non-spherical particles are generally involved in practical gas-particle systems.

Accurate prediction of drag force on individual particle is fundamental in understanding the mass, momentum and energy exchanges between the gas and particle phases. Many efforts have been carried out to predict the flow past a stationary particle based on the Finite Volume (FV) method. Most of these investigations were limited to low-to-moderate Reynolds numbers (i.e., $Re_p \leq 500$) for both spherical [10–12] and non-spherical particles [13–17]. For turbulent flow at high Reynolds numbers ($Re_p \geq 500$), limited work was conducted on spherical particles using direct numerical simulation (DNS) and large eddy simulation (LES) [18–20]. The whole range of spatial and temporal scales of turbulence can be resolved in the computational mesh by DNS, while large amount of computational resource is needed even at low Reynolds number [21]. LES reduces the computational cost by reducing the range of time scale and length scale via a low-pass filtering of the Navier-Stokes equation, and is an effective alternative for turbulence modeling. The computational resource required by LES is smaller than that of DNS, but is still higher than that of Reynolds-averaged Navier-Stokes (RANS). On the other hand, the Lattice Boltzmann (LB) method was applied to calculate the fluid-particle hydrodynamics force by Ladd [22,23]. The most notable feature of LB method is that the computational cost scales linearly with the number of particles. In the past 20 years, increasing effort have been carried out on flow past single particle or arrays of particles [24–27], with a focus on low or moderate Reynolds numbers (i.e., $Re_p \leq 500$).

Discrete element method (DEM) is an important and powerful tool for modeling particulate systems and the current trend is to move away from spheres toward more realistic (i.e., non-spherical) particle shapes. Accurate representation of the particle

* Corresponding authors at: Laboratory of Fundamental Science on Ergonomics and Environmental Control, School of Aeronautic Science and Engineering, Beihang University, Beijing 100191, China (D. Wen).
E-mail addresses: kzhang@ncepu.edu.cn (K. Zhang), d.wen@leeds.ac.uk (D. Wen).

http://dx.doi.org/10.1016/j.apt.2017.03.018
0921-8831/

shape is fundamental for the application of DEM. Up to now, the methods for describing the shape of particle mainly include composite particles, smooth and continuous surface particles, combined surface particles, and digital particles. The advantages and disadvantages of each method have been reviewed by Zhong et al. [28] in terms of accuracy, versatility, complexity and speed. The basic concept of digital particle is that any shaped particle - including the internal structure and surface texture as well as the overall shape – can be represented by a coherent collection of voxels. The resolution depends on how accurate the shape needs to be represented in particular applications [29,30]. Compared with other methods, the digital approach is not limited to mathematically easily describable shapes as voxels can be used to represent any arbitrary shapes; and the computational cost is dependent on the total number of voxels regardless of the shape complexity.

DigiDEM was proposed by using voxels (3D pixels) to represent particles instead of spheres in many conventional DEM [31]. Since both DigiDEM and LB methods operate on the same regular lattice grids in nature, a novel approach coupling the above two methods was suggested to predict the fluid-particle interactions in fluidised beds, which is more suitable for dealing with irregular shaped particles in comparison to the existed approaches [31]. To validate the predictive ability of DigiDEM coupling with LB method, a LB implementation is investigated over a much wider range of Reynolds numbers in this study. The fluid drag acting on a particle with varied shape is represented in term of the drag coefficient. The influences of Reynolds number, particle resolution, particle shape and inclination angle on the drag coefficient are carefully analyzed, and compared with the experimental data and empirical correlations published in the literature.

2. Drag correlation of single spherical/non-spherical particle

Numerous efforts have been focused on the fluid drag on a spherical particle to obtain an appropriate correlation [32–34]. Most of the drag coefficient values were obtained by particle settling experiments at low Reynolds number and by wind tunnel experiments at high Reynolds number [25]. Several correlations for the spherical particle have been proposed with different accuracies and ranges of applicability [35]. Based on a critical review of the published data, Clift et al. [36] proposed a correlation consisting 6 polynomial equations with 18 fitted constants, which shows better goodness of fit to 408 experimental data reported in the literature. After reviewing experimental studies about the fluid drag on a spherical particle since the beginning of 20th century, Brown and Desmond [35] confirmed that the correlation by Clift et al. [36] is the best for drag coefficient for spheres, despite of the slight discontinuities at some transition points from one Reynolds number range to another.

The shape diversity adds difficulties in estimating the fluid-particle interaction [37]. Holzer and Sommerfeld [38] plotted the experimental drag coefficients versus Reynolds numbers for spheres, disks and plates, lengthwise spheroids and streamline bodies, isometric particles (e.g., cubes, tetrahedrons and octahedrons) and some irregular shaped particles. It was observed that the particle shape had a strong influence on the profile of drag coefficient. Generally, the correlations for spherical particles were not valid for non-spherical particles due to the strong dependence of drag coefficient on the shape. Up to now, several drag correlations for non-spherical particles have been proposed from the experimental data [33,38,39]. Haider and Levenspiel [33] proposed a generalized correlation to associate the drag coefficient with the Reynolds number for spherical and non-spherical particles, and the so-called sphericity was introduced to describe the effect of particle shape. Ganser [39] assumed that each isolated particle experiences a Stokes's regime where drag was proportional to velocity, and a Newton's regime where drag was proportional to the square of velocity, and then developed correlations for both spherical and non-spherical particles correspondently. A simple correlation taking into account the particle orientation was established for the drag coefficient based on a large number of experimental data in the literature [38]. The mean relative deviation between this correlation and 2061 experimental data for different shapes was 14.1%, which was much lower than those of 383% and 348% from the correlations of Haider and Levenspiel [33] and Ganser [39], respectively. The simulated results are compared with the commonly used correlations for spherical and non-spherical particles, as list in Table 1.

3. Mathematical model and numerical method

3.1. Lattice Boltzmann method

Compared to the traditional CFD method that solves the Navier-Stokes equation for the macroscopic fluid dynamics, i.e. pressure and velocity, the LB method can be used to simulate fluid flow in terms of the particle distribution function, which exists at each of the grid nodes that make up the fluid domain [40,41]. The particle distribution functions relate the probable amount of fluid particles moving with a discrete speed in a discrete direction at each lattice node and each time increment. These functions are analogous to the continuous, microscopic density function of the Boltzmann equation [42]. For the LB method, time and space coordinates are discretized with velocity range in phase space limited to a finite set of vectors that represent the directions in which the fluid particles can travel. The D3Q19 model is employed in this study, as shown in Fig. 1. It has 18 discrete lattice velocities with one at rest. Components of D3Q19 lattice are listed in matrix as

$$C_i = c\begin{bmatrix} 0 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 & 1 & 1 & -1 & -1 & 0 & 0 & 0 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 1 & 1 & -1 & 1 & 1 & 1 & -1 & -1 \end{bmatrix} \tag{1}$$

Basic LB method algorithm involves the streaming and collision processes at each node and each time step: streaming process propagates particle distribution function value between neighboring nodes (Eq. (2)); collision process redistributes the functions that arrive at each node (Eq. (3)), as expressed:

$$f_i(x + c_i\Delta t, t + \Delta t) = f_i^*(x, t) \tag{2}$$

$$f_i^*(x, t) = f_i(x, t) + \Omega_i(f(x, t)) \tag{3}$$

where Δx is the lattice spacing, Δt is the explicit time step, $f_i^*(x,t)$ and $f_i(x,t)$ are the post-collision and pre-collision distribution functions, respectively. $\Omega_i(f(x,t))$ is the collision operator, it controls the relaxation rate of particle distribution function.

The relaxation process of the LB method acts on the non-equilibrium part of the distribution functions at a node to drive them toward equilibrium. The single relaxation time collision operator, Bhatnagar-Gross-Krook (BGK) model, is written as

$$\Omega_i(f(x,t)) = -\frac{1}{\tau}\left[f_i(x,t) - f_i^{(eq)}(x,t)\right] \tag{4}$$

where τ is the relaxation time and it controls the rate at which the distribution functions relaxes toward the equilibrium value; fluid viscosity is dependent on this relaxation parameter and is computed as follows