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Evaluation of drag correlations using particle resolved simulations of spheres and ellipsoids in assembly

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ABSTRACT

Particle-resolved simulations are performed to study the momentum transfer in flow though fixed random assembly of non-spherical particles. Ellipsoidal particles with sphericity ($\psi = 0.887$) are investigated in a periodic cubic domain to simulate an infinite assembly. The incompressible Navier-Stokes equations are solved using the Immersed Boundary Method (IBM). Pressure and viscous force on each particle are calculated based on the resolved flow field. Flow through an assembly of spherical particles is tested, and predicted drag forces are compared with previous particle resolved simulation results to validate the current framework. The assembly of ellipsoidal particles is simulated for solid fraction between 0.1 and 0.35 using 191 to 669 particles, respectively, at low to moderate Reynolds numbers ($10 \le Re \le 200$). The simulation results show that the drag force of ellipsoidal particles is 15% to 35% larger than equal volume spherical particles. Widely used drag force correlations are evaluated based on the current simulation results. The comparisons show that for ellipsoidal particles over the range of parameters investigated in the present study, the combination of Tenneti et al.'s correlation with Holzer's single non-spherical particle drag model has the best performance with an average difference of 7.15%.
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1. Introduction

Gas-solid flow is fundamental to many industrial processes such as pollution control, CO2 capture, biomass gasification, chemical reactors, sprays, pneumatic conveying, etc. Extensive experimental and numerical studies have been devoted to understand the interphase momentum transfer in such flows during the last several decades. Most of the studies have focused on spherical particle shapes to simplify the challenge of understanding the flow and particle characteristics. However in most natural and industrial processes, the particle shape is seldom spherical. In fact, particle shape is one of the important parameters that can have a significant impact on momentum, heat and mass transfer, which are fundamental to all processes. Although these effects of particle shape have already been widely recognized, only a few studies have been carried out to quantity them.

Most research on drag coefficient for non-spherical particle have focused on a single isolated particle. Yow et al. [1] collected experimental data of drag coefficient for a wide range of shapes including spheres, cube octahedrons, octahedrons, cubes, tetrahedrons, discs, cylinders, rectangular parallelepipeds and others. By studying the variation of drag coefficient against Reynolds number for different non-spherical particles, they showed that as the sphericity decreased, the drag coefficient increased significantly. Consequently, several drag correlations have been developed based on experimental data, using particle shape and Reynolds number as parameters. Chhabra et al. [2] studied correlations for estimating the drag coefficient of non-spherical particles in incompressible viscous fluids. 1900 experimental data points from 19 independent studies were used to evaluate the accuracy of five correlations, including those proposed by Haider and Levenspiel [3], Ganser [4], Chien [5], Hartman et al. [6] and Swamee and Ojha [7]. They found that the correlation developed by Ganser, which uses the equivalent spherical diameter and the sphericity as the particle shape parameters, performed the best. The average error from this method was 16%, though the maximum error was as high as 180%. Holzer and Sommerfeld [8] developed a general drag correlation which depends on particle sphericity, Reynolds number, and particle orientation. Comparing to 2061 experimental data points, they showed that the new correlation had a mean relative deviation of 14.1%. After performing experimental measurements of the terminal velocities of irregular particles falling in fluids, Dioguardi and Mele [9] proposed a drag correlation using sphericity and circularity as shape factors. They found the new correlation is able to predict the terminal velocity with about 11% error when the Reynolds number is known. Using a similar experimental setup, Dioguardi et al. [10] proposed another shape-dependent drag coefficient and integrated in to the multiphase code MFIX-DEM. Bagheri and Bonadonana [11] recently proposed a general model for prediction drag coefficient for non-

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spherical particles for Reynolds number up to 3×10^5 based on experimental data. Instead of using the sphericity, this new correlation uses two shape factors based on the particle flatness and elongation, and diameter to quantify the shape of the particles. The authors state that the new correlation has an average error of ~10%, which is significantly lower than existing correlations.

Compared to the rich database and correlations available for drag of an isolated particle, only a few studies focusing on drag coefficient of packed non-spherical particles have been carried out. Nemec and Levec [12] demonstrated that the original Ergun equation [13] is only able to predict the pressure drop in flow over spherical particles, whereas it systematically under-predicts the pressure drop in flow over non-spherical particles. They proposed that the dimensionless form of the Ergun equation, developed by Niven [14] with two constant factors, which only vary for different particle shapes, should be used for non-spherical particles. They conclude that with their modifications, the Ergun equation is able to predict pressure drop in flow through a packed bed of certain non-spherical particles within 10% error. However, there is no correlation to calculate the constants for arbitrary particle shapes, leaving that determination to experiments or particle resolved simulations. Moreover, the original Ergun equation significantly over-predicts the average drag force at low solid volume fractions [15], and hence the modified equation applied to a dilute system of non-spherical particles has not been validated. Machač and Dolejš [16] investigated the pressure drop in flow through a random fixed bed of non-spherical particles. They suggested that a 'bed factor' which contains the information of the non-spherical particle surface area is needed to accurately predict the pressure drop. Hua et al. [17] studied the combined Ganser and Ergun correlations and modified Syamlal and O′ Brien drag models in Eulerian-Eulerian CFD framework for irregular shape in dense gas-solid fluidized beds. Dorai et al. [18] examined the local packing structure of fixed bed reactors made of cylindrical pellets packed in cylindrical tubes. They found that the local packing structure (particle orientation) is strongly affected by the particle size distribution. Zhou et al. [19] studied packed ellipsoidal particles in a fluidized bed using CFD-DEM simulations. The drag model developed by Holzer et al. [8] was used for the ellipsoids. They concluded that the accuracy and applicability of current correlations is questionable, and a general and reliable correlation to determine fluid drag on non-spherical particles is urgently needed. Vollmari et al. [20] investigated the pressure drop in packing of arbitrary shaped particles using CFD-DEM and experiment. Based on experimental measurements, they suggested that particle drag in DEM simulations should be calculated combining the correlations developed by Holzer et al. [8] and De Felice [21]. They recommend fully resolved simulations to understand the effects of inhomogeneous packing on fluid flow structure introduced by the non-spherical particle shape.

All these studies demonstrate that further investigation is needed to have a better understanding of flow through an assembly of non-spherical particles. Therefore, in this study, particle-resolved simulations are carried out to investigate momentum transfer for a random assembly of non-spherical particles. In this approach, fluid force on each particle is calculated by resolving the flow field around each individual particle. Ellipsoidal particles with aspect ratio of 2.5 are used and the particle-fluid boundaries are resolved using an Immersed Boundary Method (IBM). The objectives of the current study are: (1) validate the current particle resolved simulation framework by comparing results for flow through spherical particle assemblies to existing drag correlations; (2) simulate flow through an assembly of ellipsoids and extract the drag force; (3) evaluate the performance of existing drag correlations for the non-spherical particles.

2. Numerical method

All simulations are performed using an in-house code – Generalized Incompressible Direct and Large Eddy Simulation of Turbulence (GenIDLEST). The details of the framework and methodology used in GenIDLEST can be found in Tafti [22] and Tafti [23]. In this section, the relevant governing equations and the modified treatments of the governing equations under fully-developed flow conditions are presented along with some details of the Immersed Boundary Method [24]. GenIDLEST with immersed boundary method has been successfully applied to oscillating cylinders [24], turbine cooling passage heat transfer [25], and fluid structure interaction problems [26].

2.1. Governing equations and numerical technique

The non-dimensional form of the Navier-Stokes equations for incompressible flow are as follows:

Continuity:

$$\frac{\partial u_i}{\partial x_i} = 0 \tag{1}$$

Momentum:

$$\frac{\partial u_i}{\partial t} + \frac{\partial (u_j u_i)}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{1}{Re_{ref}}\left(\frac{\partial^2 u_i}{\partial x_j \partial x_j}\right) \tag{2}$$

where the non-dimensionalizations are:

$$x_i = \frac{x_i^*}{L_{ref}^*}; u_i = \frac{u_i^*}{u_{ref}^*}; t = \frac{t^* u_{ref}^*}{L_{ref}^*}; P = \frac{P^* - P_{ref}^*}{\rho_{ref}^* u_{ref}^{*2}} Re_{ref} = \frac{\rho_{ref}^* u_{ref}^* L_{ref}^*}{\mu_{ref}^*}$$

The above governing equations are transformed to generalized coordinates, and discretized in a conservative finite-volume formulation using a second-order central (SOC) difference scheme on a non-staggered grid topology [27]. Cartesian velocities, pressure and temperature are calculated and stored at the cell center, whereas fluxes are calculated and stored at cell faces. A projection method using second order predictor-corrector steps is used for the time integration of the continuity and momentum equations. In the predictor step, an intermediate velocity field is calculated; and in the corrector step, an updated divergence free velocity is calculated at the new time-step by solving a pressure-Poisson equation.

2.2. Fully developed calculations

The computational domain consists of a three-dimensional periodic box representing an unbounded particle assembly. Flow is induced along the x-direction by applying a constant mean pressure gradient to balance the form and friction losses, and the total pressure is expressed in terms of the mean pressure and a fluctuating or periodic component as shown in Eq. (3).

$$P\left(\vec{x}, t\right) = -\beta \cdot x + p\left(\vec{x}, t\right) \tag{3}$$

where β is a constant. Because the applied pressure gradient will balance the form and friction losses when the flow reaches a steady state, the actual value used for β is not of any consequence to the calculated forces as long as the mean Reynolds number obtained from the simulation is the same.

With the unchanged continuity equation, the momentum equation can be written as:

$$\frac{\partial u_i}{\partial t} + \frac{\partial (u_j u_i)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{1}{Re_{ref}}\left(\frac{\partial^2 u_i}{\partial x_j \partial x_j}\right) + \beta \vec{e}_x \tag{4}$$

The $\beta \vec{e}_x$ in Eq. 4 is the mean applied pressure gradient source term, which balances the mean form and friction losses in the flow direction.

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