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Original Research Paper

Numerical investigation of effects of particle shape on dispersion in an isotropic turbulent flow

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ABSTRACT

To investigate the effects of particle shape on the dispersion in an isotropic turbulent flow, herein two direct numerical simulations are performed. The six degrees of freedom motion of spherical and spheroidal particles in a vertical uniform flow and a gas-particle two-way isotropic turbulent flow. The former, which is investigated using a numerical simulation with the Arbitrary Lagrangian-Euler (ALE) method, shows that a spheroidal particle travels with rotating and oscillating motions, which significantly affect the pressure and the friction force on the particle's surface. The trend of the fluid force acting on the spheroidal particle's surface also oscillates and differs from that on a spherical particle. The time variation of the fluid force on the spheroidal particle is modeled in the C_D equation, which has a sine curve's PDF relation with Re_p and the particle's maximum and minimum C_D values. The latter simulation examines the effects of the particle shape on the dispersion with the motion model developed above. The particle's dispersion behavior, which is analyzed by the statistical variable D and the Radial Distribution Function (RDF), shows that the dispersion motion is markedly affected by particle's sphericity, especially for particles with a relatively small sphericity. The results suggest that this difference can influence ignitability, flammability, and the concentration of combustible gases released by particles, and requires further study.

1. Introduction

Industrial applications around the world utilize gas-particle two-phase flows. For instance, in coal-fired power plants, which are one of the largest industries in terms of power production and CO_2 emission, there is an urgent need to realize clean coal technology to reduce the CO_2 emission. It is important to achieve a much deeper understanding of the two-phase reacting fields on pulverized coal combustion boilers or coal gasifiers, which consume a great amount of coal. However, pulverized coal combustion is a complex phenomenon. The underlying physics governing the simultaneous and interactive dispersion, evaporation, and devolatilization of pulverized coal particles, as well as the heterogeneous and homogeneous reactions are not well understood. For such a flow, Computational Fluid Dynamics (CFD) is frequently used. Watanabe and colleagues [1–6] have performed numerical simulations of pulverized coal combustion and gasification on a wide range of reactor scales and investigated the detailed behavior of coal flames.

Many types of research in the coal combustion field assume that coal particles are spherical, simplifying the numerical problems and reducing the computational cost, but particles prepared by a pulverizer have non-spherical shapes. This assumption, which neglects the real shape of coal particles, is not well assessed and a detailed discussion about the simplification in the literature is limited. Many efforts have been done to investigate the non-spherical particle's behavior, and spheroidal particles are frequently used, such as Feng et al. [7], Broday et al. [8], Mortensen et al. [9]. These works are slowly beginning to unravel the motion characteristics of a spheroidal particle, but they mainly focused on the behavior of a single spheroidal particle's motion. Also, many works were done to model the complex motion behavior of the non-spherical particle. Haider and Levenspiel [10] proposed the drag curve characterized by sphericity of a particle. Hlzer and Sommerfeld [11] suggested a formula for drag coefficient by using the normal, crosswise, and lengthwise sphericities. Rosendahl [12] developed a multi-parameter drag coefficient correlation and Zastawny et al. [13] expanded it. These works modeled the drag coef-

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ficient, which usually is the dominator of the motion. Mando et al. [14] discussed the aspects of modeling the motion of non-spherical particles, and Voth et al. [15] reviewed the most of the strategies of large particle and point-wise regime simulation.

Here in this study, numerical simulations with six degrees of freedom motion of a single spherical or spheroidal particle are initially performed by employing the Arbitrary Lagrangian-Eulerian (ALE) method. We numerically investigated the drag coefficient curve of the particle. And then as the first stage, we modeled the drag coefficient with its probability density function (PDF) by a practical view. Finally, the motion model developed here is introduced into a computation of a gas-particle two-phase isotropic turbulent flow to investigate the dispersion characteristics of non-spherical particles in a turbulent flow. The results are compared to the behavior of spherical particles.

2. Analysis and modeling of the motion of a single non-spherical particle

In this section, the motion characteristics of single non-spherical particles are examined and modeled by a numerical simulation with six degrees of freedom motion.

The well-known Basset-Boussinesq-Oseen equation (B.B.O equation), which is valid for a spherical particle moving in a fluid, is expressed as

$$\rho_p V_p \frac{d\boldsymbol{v}}{dt} = \boldsymbol{F}_D + \boldsymbol{F}_L + \boldsymbol{F}_B + \boldsymbol{F}_{prs} + \boldsymbol{F}_{mass} + \boldsymbol{F}_{Basset}, \tag{1}$$

where ρ_p, V_p and $\boldsymbol{v}$ are the density, volume, and velocity of the particle, respectively. $\boldsymbol{F}_D, \boldsymbol{F}_L, \boldsymbol{F}_B, \boldsymbol{F}_{pre}, \boldsymbol{F}_{mass}$, and $\boldsymbol{F}_{Basset}$ are the drag force, lift force, buoyancy, pressure gradient, virtual mass, and Basset history term, respectively. Because the drag force mainly contributes to the motion of a particle in a pulverized coal combustion field, this study pays special attention to it. The drag force can be calculated by summing the contributions of friction and pressure as

$$\boldsymbol{F}_D = \boldsymbol{F}_{Dprs} + \boldsymbol{F}_{Dfrc} = -\int_S p\boldsymbol{e}_y \cdot \boldsymbol{n} dS + \int_S \boldsymbol{n} \cdot \boldsymbol{\tau} \cdot \boldsymbol{e}_y dS, \tag{2}$$

where $\boldsymbol{n}$ is the surface normal vector, τ is the stress tensor, and $\boldsymbol{e}_y$ is the particle's direction of motion relative to the ambient fluid flow. Although Eq. (2) can be used for any particle, Eq. (1) is only strictly valid for spheres.

The drag coefficient C_D is defined as

$$C_D = \frac{\boldsymbol{F}_D}{\frac{1}{2}\rho_f|\boldsymbol{u} - \boldsymbol{v}|^2 A} = C_{Dprs} + C_{Dfrc}, \tag{3}$$

where ρ_f and $\boldsymbol{u}$ are the fluid density and velocity, respectively. A is the projection area of the particle to the flow direction. C_D can also be divided into C_{Dprs} and C_{Dfrc}, which are influenced by the friction and the pressure, respectively. C_D for a spherical particle can be plotted as a function of the Reynolds number Re_p, and many works try to propose an equation to express the curve. Clift et al. summarized some of the most popular expressions [see 16, p. 111] and provided the following recommendation

$$C_D = \begin{cases} 3/16 + 24/Re_p, & Re_p < 0.01 \\ \frac{24}{Re_p}(1 + 0.1315 Re_p^{0.82 - 0.05 * \log_{10} Re_p}), & 0.01 < Re_p \le 20 \\ \frac{24}{Re_p}(1 + 0.1935 Re_p^{0.6305}), & 20 \leqslant Re_p < 260 \end{cases} \tag{4}$$

where the Re_p is based on the slip velocity and particle size

$$Re_p = \frac{\rho_f|\boldsymbol{u} - \boldsymbol{v}|d}{\mu}, \tag{5}$$

here d is the diameter of the particle and μ is the viscosity of the fluid, respectively.

Eqs. (1) and (4) are only suitable for spherical particles. These equations must be modified for non-spherical particles. Haider and Levenspiel [10] studied C_D of non-spherical particles by investigating the relations between C_D, Re_p and sphericity. They proposed a design chart of C_D with the sphericity dependence.

Sphericity is defined as the ratio of the surface area of a sphere to the surface area of a given particle where the sphere and the given particle have the same volume as

$$\phi = \frac{S_{sphere}}{S_{particle}} = \frac{\pi^{\frac{1}{3}}(6V_{particle})^{\frac{2}{3}}}{S_{particle}}. \tag{6}$$

According to Haider & Levenspiel, C_D becomes larger as the sphericity becomes smaller.

2.1. ALE method

To consider the six degrees of freedom for a particle's motion, the Arbitrary Lagrangian-Eulerian (ALE) method [see 17,18, chapter 14] is employed. The governing equations of the ALE method are

$$\frac{\partial \rho_f}{\partial t} + ((\boldsymbol{u} - \boldsymbol{u}') \cdot \nabla)\rho_f = -\rho_f \nabla \cdot \boldsymbol{u}, \tag{7a}$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + ((\boldsymbol{u} - \boldsymbol{u}') \cdot \nabla)\boldsymbol{u} = -\frac{1}{\rho_f}\nabla p + \frac{1}{\rho_f}\nabla \cdot \boldsymbol{\sigma} + \boldsymbol{g}, \tag{7b}$$

$$\frac{\partial h}{\partial t} + ((\boldsymbol{u} - \boldsymbol{u}') \cdot \nabla)h = \frac{1}{\rho_f}\nabla \cdot (D_h \nabla h). \tag{7c}$$

where ρ_f and $\boldsymbol{u}$ are the fluid density and velocity, respectively, $\boldsymbol{u}'$ is the mesh velocity, p is the pressure, $\boldsymbol{\sigma}$ is the surface stress tensor, D_h is the enthalpy diffusion coefficient, and h is the total enthalpy. The ALE method is equivalent to the Lagrangian method when $\boldsymbol{u}' = \boldsymbol{u}$ but is equivalent to the Eulerian method when $\boldsymbol{u}' = 0$. We apply a particle's velocity $\boldsymbol{v}$ to $\boldsymbol{u}'$. Thus the slip velocity $\boldsymbol{u} - \boldsymbol{v}$ is generated between a fluid and a particle, which depends on the pressure and friction force distributions on the particle's surface. This means that the entire mesh around a single particle rotates and oscillates due to the variations in the pressure and friction force distributions. The six degrees of freedom motion of a particle in a fluid flow can be performed by this procedure.

In order to obtain the particle's velocity, the motion of the single particle is calculated. The governing equation of a rigid body is

$$m\frac{d^2\boldsymbol{z}}{dt^2} = \boldsymbol{F}, \tag{8a}$$

$$\boldsymbol{I}\frac{d^2\boldsymbol{\alpha}}{dt^2} + \frac{d\boldsymbol{\alpha}}{dt} \times \left(\boldsymbol{I}\frac{d\boldsymbol{\alpha}}{dt}\right) = \boldsymbol{M}. \tag{8b}$$

m and $\boldsymbol{I}$ are the mass and moment of inertia of particle. z and $\boldsymbol{\alpha}$ are the displacement and rotation angle, respectively. $\boldsymbol{F}$ and $\boldsymbol{M}$ are the force and torque on the particle, which are obtained by considering the integration of the fluid force over the surface and the gravity. Subsequencely we can calculate the moving and angular velocities of the particle, and apply them to Eqs. 7a, 7b, and 7c of the ALE method.

2.2. Validation of the DNS with ALE method

Here we validated the DNS with ALE method.

Firstly, we calculated a spherical particle's C_D values and compared them to the empirical Eq. (4). The particle was moving freely in a uniform flow and its instantaneous Reynolds number Re_p and C_D values were extracted and examined. The spherical particle of case SV shown in Table 3 was used. This study aimed to investigate the motion of tiny non-spherical particles, such as pulverized coal particles in a pulverized coal combustion system or a coal gasifier.