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On the accuracy of Lagrangian point-mass models for heavy non-spherical particles in isotropic turbulence

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ABSTRACT

The interaction of isotropic turbulence with heavy particles, the size of which is on the order of the smallest turbulent eddies, is considered. Although this case is relevant to pulverized coal and biomass combustion, there is an apparent lack of reliable numerical models for the particle dynamics and the response of the turbulent flow field. By conducting particle resolving direct numerical simulations, we generate accurate results for the dynamics of spherical and non-spherical particles and the associated turbulence modulation effects. Subsequently, we verify the ability of two different two-way coupled Lagrangian models, one derived for spherical and one for ellipsoidal particles, to reproduce the reference results. It is found that the velocities of prolate ellipsoids are significantly reduced compared to spherical particles of the same volume. This behavior is captured by neither of the Lagrangian models since the spherical model does not account for the particle shape and the ellipsoidal model does not account for particle inertia. Additionally, the spectra of fluid kinetic energy indicate that the models fail to resolve the interaction in the high wave number regime, i.e., the interaction of the particle boundary layers and wakes with the smallest flow scales. This is reflected by the vast underprediction of the overall viscous dissipation by both models. As a consequence, the attenuation of kinetic energy contained in large-scale flow structures is underpredicted by the Lagrangian models. In summary, for the slightly non-spherical particles, accounting for inertia effects appears to be more important than inclusion of non-spherical effects for the kinetic energy balance of both phases. However, the ellipsoidal particle model reproduces the preferential alignment of the non-spherical particles within the turbulent flow which becomes more important in highly anisotropic turbulent flows such as in industrial furnaces.

1. Introduction

Turbulent flows interacting with suspended particles of complex shape are encountered in numerous technical and natural processes, such as pulverized fuel combustion, composite material production, pollutant transport in the atmosphere and hydrosphere, blood flow, or the deposition of dust in the human airways. Due to the disparity of the involved length and time scales, a full resolution of the dispersed phase by numerical simulations is beyond todays computational capabilities for practical applications. The development of reliable models for the muliphase dynamics is challenging due to the shape- and size-dependent particle motion and their complex interaction with the typically turbulent carrier phase. Therefore, these models are usually derived under simplifying assumptions such as very small particle diameters and strictly spherical particle shapes.

It goes without saying that sphericity is an idealized particle property which is not found in real applications. Nonetheless, it is a widespread assumption in numerical simulations of multiphase systems, since it simplifies modeling attempts significantly. Whereas the importance of particle anisotropy has been emphasized in studies of biomass combustion [1,2], ice-crystal formation in atmospheric clouds [3], papermaking [4], or the locomotion of microorganisms [5], it is commonly considered negligible in pulverized coal combustion. Moreover, the characteristic shape distribution of pulverized coal particles has rarely been quantified in the literature. Mathews et al. [6] report a mean aspect ratio, defined as the ratio of maximum to minimum particle extent, of 1.7 for pulverized bituminous coal with a significant variation of the samples including much larger aspect ratios. More importantly, they report an underestimation of the characteristic heating time by 22% and terminal velocities by 20% if the particle shape was neglected. Sim-

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ilarly, Maloney et al. [7] found a significant underestimation of the heating rates by 50% during coal particle heating and devolatilization where the neglected shape effects were concluded a potential reason.

The main assumption in deriving Lagrangian point-particle models is that the particle diameters be small compared to the local characteristic length scale of the flow, $d_p \ll l_c$. However, in simulations of industrial scale, this condition can hardly be verified neither circumvented. This is attributed to the difficulty of measuring or predicting flow scales in technical flows, i.e., for strongly inhomogeneous turbulence on the one hand and to a lack of alternatives for modeling the particle phase on the other hand. For combustion or gasification of pulverized coal, even in studies of lab-scale facilities only a few quantify the Kolmogorov or integral length scales [8] of the turbulent flow field in the vicinity of the injectors feeding the particles or in the flame-front regions. Recent studies on particle-laden coaxial jets [9], swirl jet burners [10], and coal gasifiers [11] report Kolmogorov length scales on the order of $\eta = \mathcal{O}(50\text{–}100\ \mu\text{m})$. This is in agreement with measurements on turbulent swirl jets [12] where $\eta = \mathcal{O}(30\ \mu\text{m})$ was observed. Since typical coal particle size distributions are considered in the range $d_p = 30\text{–}100\ \mu\text{m}$ [6,1], at least in the near-nozzle areas one has to consider that $d_p \sim \eta$ when applying numerical models for the two-phase turbulent flow. For industrial-scale pulverized coal-fired burners, scaling laws obtained for turbulent jet flows can be considered for an order-of-magnitude estimate of the local flow scales. The studies by Antonia et al. [13] and Rowinski and Pope [14] indicate that in the centerline region of single jet flow and in the outer shear layer region of coaxial jets there exists a $\eta/D \sim Re^{-3/4}$ scaling where D is the jet diameter and Re is the jet Reynolds number. This relation illustrates that the growth of the characteristic length scales with the facility dimensions is compensated by the increasing separation between the smallest and the largest scales, i.e., by an increasing bandwidth of scales with growing Reynolds number. Thus, the condition $d_p \ll \eta$ remains at least questionable for both lab- and industrial-scale pulverized coal combustion. However, while the cases $d_p \ll \eta$ and $d_p \gg \eta$ of particulate turbulent flow have been intensively studied in the literature, the intermediate particle sizes $d_p \sim \eta$ were seldomly analyzed as they are challenging for experimental and numerical methods. A recent study on the turbulence modulation at $d_p \sim \eta$ via particle resolved simulations [15] indicates that heavy particles strongly influence the level of kinetic energy and viscous dissipation close to the particle surfaces which is not resolved by standard particle models. That is, the efficacy of point-mass models is not known in this setting.

In this study, we investigate the accuracy of Lagrangian point-particle models for the simulation of spherical and slightly non-spherical particles with sizes on the order of the smallest scales of the fluid motion. Accurate reference results are computed by a recently developed numerical method for direct particle-fluid simulations (DPFS) of turbulent flows [16]. In these simulations, in addition to the smallest scales of the turbulent fluid motion, the particle boundary layers and wakes are resolved by using locally refined meshes. Since the solution scheme conserves mass, momentum, and energy [16], it is ideally suited to investigate the turbulence modulation by the particles and the associated particle response. Subsequently, the same configuration is simulated using two different Lagrangian point-particle schemes developed for spherical [17] and ellipsoidal [18,19] particles. A direct comparison of the different results will be conducted to assess the solution quality of the Lagrangian schemes under the given conditions. Based on the results of the three different methods, we seek to answer the following questions.

- How accurate are two-way coupled Lagrangian point-particle models when the particle diameter is on the order of the smallest scales of the turbulent flow?
- How accurate are spherical particle models when applied to configurations involving non-spherical particles?
- Can these models accurately predict the exchange of kinetic energy between the dispersed and the carrier phases, i.e., the turbulence modulation?
- At which scales of the fluid motion does the interaction with the particles occur?

The latter question has important implications for large-eddy simulations (LES) of particulate turbulent flows. In these simulations, a potential interaction of the unresolved, i.e., subgrid scales of the turbulent velocity fluctuations, with the flow field disturbances by the particles has to be accounted for. That is, when applying Lagrangian point-particle models, a model-to-model two-way coupling with the subgrid scheme is required. In LES studies of pulverized fuel combustion, the influence of subgrid scale velocity fluctuations on the particles is either neglected [20] or included via stochastic models [21]. However, when $d_p \sim \eta$ more sophisticated models might be required to model the reverse coupling of the particles to the subgrid fluctuations.

The purpose of the present study is the fundamental analysis of the particle dynamics and the fluid-particle interaction in a generic turbulent flow field. That is, the results apply to various turbulent dispersed multiphase flows. In particular, the parameter range is chosen to resemble the conditions observed in pulverized coal combustion facilities and motivated by the substantial uncertainties which are encountered in state-of-the-art models for the simulation of pulverized coal and biomass combustion. We emphasize that assessing the accuracy of particle and turbulence models in real burner geometries can merely provide evidence for the specific configuration. The complex interaction of, e.g., the anisotropic flow structure, the chemically reacting flow field, devolatilization, thermal radiation, and particle collisions, strongly influence the understanding of the origins of the modeling errors. Thus, the present study is considered a first step to understand the dynamics of pulverized coal particles in real flows, that is, to identify the impact of the particle shape and the particle size on the coupled dynamics in an isotropic turbulent flow field, with and without gravity. Nonetheless, the results for the particle dynamics and the turbulence modulation have direct consequences for the particle residence times and therefore are closely connected to the conjugate heat transfer, surface reactions, devolatilization, thermal radiation, or particle collisions.

The paper is organized as follows. In Section 2 the governing equations of the multiphase system are given. The numerical method is presented in Section 3, including a description of the fluid-particle coupling strategy in the particle resolved simulations and in the Lagrangian point-mass schemes. The results for the turbulence modulation by the particles and the particle dynamics obtained with the different methods are discussed in Section 4. Finally, concluding remarks are given in Section 5.

2. Equations governing particle-laden viscous flow

2.1. Viscous fluid flow

The motion of a viscous compressible fluid in the time-dependent domain $\Omega_f(t)$ is considered. The conservation of mass, momentum, and energy in a moving control volume $V(t) \subset \Omega_f(t)$ in non-dimensional arbitrary Lagrangian-Eulerian formulation [22] reads