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A simplified two-fluid model coupled with EMMS drag for gas-solid flows

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ABSTRACT

A simplified two-fluid model (STFM) combined with energy-minimization multi-scale (EMMS) drag was proposed for accurate and fast simulation of gas-solid flows. In the proposed approach, the solid phase viscosity is neglected, the solid phase pressure is calculated with an empirical formulation, and the interphase momentum transfer is modeled with EMMS drag, which takes the effects of meso-scale structures into consideration. Three typical fluidization cases, namely, a 2D circulating fluidized bed, a 3D lab-scale bubbling fluidized bed, and a 3D lab-scale full-loop circulating fluidized bed, were successfully simulated with this approach. The numerical results are compared with those of full two-fluid model (FTFM, i.e., the two-fluid model using the kinetic theory for granular flow to close solid phase stress term), as well as experimental data. Predictions of STFM coupled with EMMS drag are comparable with those of FTFM coupled with EMMS drag, and both agree well with experimental data. However, computational cost of STFM is significantly reduced compared with that of FTFM. It is suggested that drag model has a dominant effect on gas-solid simulation, and the effect of solid phase stress term seems to play a minor role, demonstrating the feasibility and practicality of STFM with EMMS drag for describing the hydrodynamics of heterogeneous gas-solid flows.

1. Introduction

Gas-solid two-phase flows are widely encountered in many chemical engineering and energy conversion industries. Over the past decades, computational fluid dynamics (CFD) has been playing a more and more important role in predicting hydrodynamic behaviors of these systems, which are critical to the design, scale-up, and optimization of those industrial units. However, accurate and fast simulation of gas-solid systems is hindered by their inherent heterogeneity at the meso-scale in a computational grid [1,2]. For example, in a circulating fluidized bed, gas-solid flow features intrinsically heterogeneous and dynamical structures with scales ranging from single particle scale to vessel scale [3–5]. Meso-scale structures, such as particle clusters, which is a result of inherent inter-particles forces overcoming the hydrodynamic forces, have profound influence on the flow behaviors [3, 4,6–15]. To date there is no agreement on appropriate closure models for those complex structures [13]. Existing constitutive models for interphase momentum transfer are mostly semi-empirical. In fact, there is still no agreement on the governing equations [13].

1.1. Two-fluid model

Generally speaking, CFD models for gas-solid flows can be classified into three levels [16]: direct numerical simulation (DNS) [17–25], discrete particle model (DPM, also known as Eulerian-Lagrangian model) [26–30] and two-fluid model (TFM, also known as Eulerian-Eulerian model) [31–33]. DNS is the most fundamental and accurate approach, in which each single particle is fully resolved and tracked according to the Newton's law, and particle-particle and particle-wall interactions are modeled either with hard sphere model [26,34] or discrete element method (DEM) [35]. Gas phase is considered as a continuum, and the grid scale for the gas phase is required to be one order of magnitude smaller than the diameter of particles. The surfaces of particles are considered as no-slip walls and flow structures around particles are fully resolved, and the forces exerted on particles can be obtained from surface integration of stresses on the surface of particles, thus no closure model is needed. In DPM, particles are tracked the same way as in DNS, gas phase is governed by volume-averaged Navier-Stokes equations, and grid size for gas phase is about an order of magnitude larger than the diameter of particles. Since the flow structures around particles are not resolved, closure models for gas-solid interphase momentum transfer are required. As a method of the highest level, two-fluid model considers both gas and solid phase as interpenetrating continuum and describes both phases in an Eulerian framework. Apart from models for interphase momentum transfer, additional closure models for particle-particle and particle-wall interactions are needed.

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In the two-fluid model, interactions between particles are considered in the form of a solid phase stress term in the solid phase momentum equation. To close the solid phase stress term, solid phase viscosity and pressure are required. Earlier researchers neglected the solid phase stress [36], or assumed that solid phase is a Newtonian fluid with a constant viscosity and correlated the solid phase pressure with physical properties of the particles and local voidage [37–39]. Whereafter, more fundamental closures have been developed, and one of the most widely used is the kinetic theory for granular flow (KTGF) model [40–43]. The KTGF model is based on the analogy of solid particles to molecules of dense gases [44]. The concept of granular temperature is introduced to quantify the energy of fluctuating motions of particles and a partial differential equation is developed to govern the transportation of granular temperature, with the aid of additional closure models for thermal conductivity coefficient [32,42,45], radial distribution function [32,42,46,47], energy dissipation due to inelastic collision between particles [41] and energy dissipation due to force exerted on particles by gas phase [48–50]. In addition, the solid phase viscosity [32,42,45,51], bulk viscosity [42] and pressure [42] are modeled as functions of granular temperature. Recently, Igci et al. [52] and Milioli et al. [53] developed a filtered two-fluid model to account for the missing effect of meso-scale structures on coarse-grid simulations. In their approach, the results of highly resolved numerical simulations based on the full set of equations are filtered to derive a coarse-grid correction formulation for drag coefficient (as well as for the solid-phase pressure and viscosity), which is a function of the grid size, solid volume fraction and scalar shear rate. However, theoretically the KTGF model is only suitable for dilute regions where particle-particle interaction is dominated by instantaneous binary collisions. For regions with densely packed particles, the interaction between particles is dominated by enduring frictional contacts involving multiple particles. To consider the frictional contacts in those dense regions, several frictional stress models [54–65] have been proposed. On the other hand, the impact of walls to the solid phase takes effect through wall boundary conditions for both solid phase momentum equation and granular temperature equation. Johnson and Jackson [58] proposed a widely used wall boundary condition, which assumes that particles partially collide with the wall and the rest slide along. The energy flux for granular temperature equation and the sliding velocity of particle phase relative to walls were modeled. In the boundary condition proposed by Johnson and Jackson, specularity coefficient should be specified to characterize tangential momentum transfer due to collisions, which lacks experimental measurement, and some researchers [66–68] reported great sensitivity of simulation results on this coefficient. Li and Benyahia [69] suggested an analytical expression for the specularity coefficient on a frictional surface and provided a method to determine it for more general problems.

1.2. Structure-dependent drag

Interphase momentum transfer model is vital for the gas-solid flow simulation, and one of the most important is the drag model [70]. Conventional two-fluid model commonly uses homogeneous drag model based on the assumption of particles being distributed homogeneously in computational grids [71,72], such as Gidaspow drag which is a combination of Wen and Yu correlation [72] and Ergun equation [71]. Homogeneous drag models have been reported to overestimate the drag force notably [11,12,73–79]. The reason is that heterogeneous distribution of particles prevails in the system and the unresolved heterogeneous structures have significant effects on drag [6,52,80–82]. To take into account those effects, many sub-grid drag models have been proposed [52,74,82–86]. EMMS-based drag models [82,84] which take into account the effects of particle clusters, have been reported to greatly improve the predictions of gas-solid flows in circulating fluidized beds, compared with those using the homogeneous models [32,71,72]. Yang et al. [79,82] are the first to adopt the structural parameters from EMMS model to correct the drag coefficient, and successful CFD simulations of riser with Geldart A particles were showed in their researches. Wang and Li [84] extended this model to the sub-grid level and thus made it adaptable to a broader range of operating conditions [76,87–92]. Recently a bubble-based EMMS model and a series of EMMS-based drags suitable for bubbling fluidized beds have been proposed [93–95], and results showed that simulation with EMMS drag obtained a much higher accuracy than those with traditional homogeneous drag model.

1.3. Solid phase stress

The influence of the solid phase stress term is minor compared with that of the drag term [36,38,39,96–98]. When solid phase stress model especially the KTGF model is involved, computational cost will be increased significantly. For instance, Bouillard et al. [36] reported that in many applications solid phase stress term was unimportant for simulation results but significantly increased computational cost. They utilized a model neglecting both gas and solid phase stress terms to simulate a bubbling fluidized bed of Geldart B particles with an immersed obstacle. Van Wachem et al. [98] investigated the influence of different governing equations and various closure models including solid phase stress models, radial distribution models and drag models, on the simulation of gas-solid systems. They found that only drag models affected solid phase flow behaviors significantly. More recently, the performances of both the constant viscosity model (CVM) and the KTGF model on bubbling fluidized beds are compared [38,39,98]. Both the CVM and KTGF model showed similar predictions on time-averaged axial porosity profiles, bubble growth rate and rise velocity of large bubbles. All the results mentioned above imply that drag may be the dominant term in gas-solid governing equations.

Furthermore, as mentioned previously, the coupling of EMMS drag with two-fluid model involving KTGF model (referred as full two-fluid model, FTFM) gained great success. However, it is worth noting that no structural parameters are considered in KTGF model, and the improvements can only be attributed to the consideration of heterogeneous structures in the drag model. This further convinces us the predominant role of the drag term, and motivates us to couple EMMS drag with two-fluid model based on simplified solid phase stress model (referred as simplified two-fluid model, STFM), which is expected to obtain similar success but with significantly reduced computational cost.

1.4. Objective

The objective of this study is to develop a simplified two-fluid model in which particle-particle interaction is considered using a simple empirical formulation and drag force is evaluated with EMMS-based sub-grid drag model, trying to demonstrate that the drag term has a dominant effect on the dynamics of gas-solid systems, and additional computational expense required for solving transport equations in the KTGF model is not always a necessity. All the development and numerical simulation were carried out under the platform of OpenFOAM [99]. The rest of this manuscript is organized as follows: firstly, the governing equations and numerical treatments of STFM are described; then numerical simulation of 2D circulating fluidized bed of Geldart A particles [100] is carried out with STFM, and the results are compared with previous research of Lu et al. [76]; furthermore, a 3D bubbling fluidized bed of Geldart A particles is simulated with FTFM and STFM respectively, and the simulation results of FTFM with homogeneous drag, FTFM with EMMS drag, STFM with homogeneous drag and STFM with EMMS drag are compared with each other as well as with experimental data; the computational costs of STFM and FTFM are also compared; finally, a lab-scale circulating fluidized bed which is part of the Virtual Process Engineering (VPE) project [101] is simulated using both FTFM and STFM coupled with EMMS drag, with results compared between these two models as well as with experimental measurements.