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Hydrodynamics of gas–solid risers using cluster structure-dependent drag model

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A modified cluster structure-dependent (CSD) drag model is proposed to improve drag predictions for heterogeneous gas–solid flows in risers. A micro-meso-grid scales (M2GS) equation set consists of six hydrodynamic equations and one stability criteria with bivariate extreme value (BEV) theory as a function of eight independent variables and four dependent parameters on the basis of grid parameters. The modified CSD drag model is further verified by CFD simulations by coupling with the two-fluid model for low and high solid fluxes in risers. The simulated results in 2D domain of the riser are compared with those using the Huilin–Gidaspow drag model and experimental data. The modified CSD drag model is verified by CFD simulations by coupling with a kinetic theory of granular flow based two-fluid model for low and high solid fluxes in risers. The comparison shows that the modified CSD drag model is able to capture the axial heterogeneity with the dense bottom and dilute top sections. The radial profiles using modified CSD drag models show only qualitative agreement with the experimental data. The results using the modified CSD drag model and Huilin–Gidaspow drag model show a reasonable agreement at the center. Thus, further improvements combining with wall friction effect are required to achieve quantitative agreement with experimental data.

1. Introduction

Extensive applications of the circulating fluidized bed (CFB) technology have become an increasingly important unit operation, with examples of principal applications including fluid catalytic cracking [1], gasification and combustion [2]. Such gas–solid suspensions are inherently unstable, leading to transient particle clusters continuously forming and breaking up [3,4]. Because clusters affect the hydrodynamics (e.g., gas–solid contact time, elutriation rate) and hence impact reactor performance (e.g., productivity, rate of reaction, heat transfer), an enhanced understanding of the behavior of such flow structures in the CFB riser is necessary.

Computational fluid dynamics (CFD) is an effective tool for understanding the fundamental hydrodynamics of gas and particles in risers. The gas–solid two-fluid model based on kinetic theory of granular flows [5] is the most widely used among the numerous numerical studies in risers. The two-fluid model is especially applicable due to its computational simplicity for risers with high volume fraction of particles. However, a major challenge for CFD models of risers is to realistically resolve the effect of clusters on the momentum exchange between the gas phase and solid phase. The clustering of particles results in a heterogeneous structure of solid phase including the dense phase of clusters and dilute phase of dispersed particles, and has a high gas–solid slip velocity and remarkable drag reduction [6]. Quantifying the clusters and their effects on the drag is critical for the realistic simulations of flow of gas and particles in risers.

Generally, the drag force acting on particles in fluid–solid systems is represented by the product of the drag coefficient β and the slip velocity (u_s–u_g) between the two phases. To date, several drag models have been developed to predict the interphase drag coefficient. A drag model which takes into account the cluster effects was proposed by O'Brien and Syamlal [7]. This model was limited to only two solid mass fluxes due to an empirical factor. A scaling factor of 0.2 to 0.3 was used to take the effect of the reduction of drag force into account due to the particle agglomeration [8,9]. This indicates that to represent the reduced drag force a scale factor applied to the standard drag law is simple and effective, but a careful adjustment should be made in the numerical simulations of fluidized beds. However, to find an appropriate scale factor, this empirical approach requires an extensive case study for every application. In order to make the kinetic theory of granular flow applicable to flow of clusters and dispersed particles in risers, the model of two granular temperatures, one for clusters and another for dispersed particles, is proposed to show the velocity fluctuations of dispersed particles and clusters [10]. The model represents the clusters as a separate phase. The distributions of velocities and granular temperatures of clusters and dispersed particles are predicted. The energy minimization multiscale approach (EMMS) developed by Li et al. [11–13] has been used to predict steady flow inside circulating fluidized beds. The EMMS drag method assumes that particles move in clusters through a dilute phase composed of the surrounding gas and a few randomly distributed particles. The clusters of dense phase and the

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dispersed particles of dilute phase consist themselves of homogeneously distributed particles enabling the application of a homogenous drag correlation to these structures. The resulting underdetermined set of equations is solved by minimizing the energy consumed by the transport of the particles, referred to as stability condition. Eight inhomogeneous structure parameters (ε_{gf}, U_{gf}, U_{sf}, f, ε_{gc}, d_c, U_{gc} and U_{sc}) are solved with the specified operating conditions (superficial gas velocity Ug and solid mass flux Gs) to close the equations of the EMMS drag model. Later, it extended its principle to the control volume of the two-fluid model and was integrated into the Eulerian formalism in the form of a drag correction by adding acceleration of particles in the dilute phase (a_f) and clusters in the dense phase (a_c) [14]. In this version of the EMMS model these ten independent variables (ε_{gf}, U_{gf}, U_{sf}, f, ε_{gc}, d_c, U_{gc}, U_{sc}, a_c and a_f) were solved by a two-step scheme. Firstly, EMMS model assumes that the meso-scale structure parameters (ε_{gc}, d_c) are determined by macro-scale operating conditions (superficial gas velocity Ug and superficial velocity of particles Us) together with a stability criterion. Secondly, the remaining independent parameters are resolved by deterministic solution of a set of non-linear conservation equations. On the other hand, additional equations to calculate a_c and a_f were proposed by Wang et al. [15] on the basis of the variance of solid concentration fluctuation. However, the validation of EMMS drag model is still a problem because the original equations stem from a global fluidized bed system, not grid cells of numerical simulations. Shah et al. [16] derived a structure-based drag model on the basis of the EMMS model. They assume the voidage of the dilute phase is to be unity ($\varepsilon_{gf} = 1.0$). This assumption implies that the dilute phase does not have particles, and the velocity of particle in the dilute phase can be equated to zero. Jiradilok et al. [17] used the drag model specified Ug = 1.52 m/s and Gs = 14.3 kg/m^{2}s from EMMS method proposed by Yang et al. [18] to simulate the flow in high solid flux risers. This was a major drawback in this study because the solution of the EMMS model depends on the flow parameters, and the drag calculated for a particular flow system cannot be used in another flow system. Benyahia [19] performed numerical simulations of flow of FCC particles (Geldart group A powder) using EMMS drag model proposed by Lu et al. [20] in a 2D circulating fluidized bed. Simulated results showed that the standard Wen-Yu drag model essentially predicted a homogeneous flow where the bed of particles was transported along the height of the riser. Simulations showed that the EMMS drag in the hydrodynamic model prompts the formation of heterogeneous flow structures that limit the circulation of particles. Simulations indicated that the grid resolution may be necessary to fully demonstrate the accuracy of two-fluid model in predicting gas–solid flows in the risers [21]. Results indicated that the subgrid corrections were needed to predict the flows in large-scale reactors. On the other hand, the filtered drag models proposed by Sundaresan group were obtained using finely resolved simulations as the computational grid was refined and more flow structures were resolved. Agrawal et al. [22] have shown that the effect of cluster structures on the macroscopic behavior for practical simulations can be taken into account by sub-grid scales through additional closure relations, which can be derived by means of a highly resolved simulation. The effective drag coefficient was measured using the highly resolved simulations of periodic flows and depended on the particle volume fraction. Using these numerical results, Igci and Sundaresan [23] constructed ad hoc subgrid models for the effects of the fine-scale flow structures on the drag force and the solid stresses, and examined the consequence of these subgrid models on the outcome of the coarse-grid simulations of gas-particle flow. The group of Simonin proposed a subgrid model for drag coefficient from filtering highly resolved simulations. Simulated results by Parmentier et al. [24] suggested that the overestimation of the drag force was linked to the existence of a subgrid drift velocity, which reduced the effective resolved slip velocity. The model depends strongly on the simulation case and the grid resolution. These filtered models mentioned above are the analog of large-eddy simulation of single-phase turbulent flow, where one simulates spatial and spatio-temporal patterns occurring at the macro-scale using the conservations of mass and momentum, but accounts for the effects of meso-scale structures occurring at a scale smaller than the grid size through additional closure relations. However, the transfer and dissipation of fluctuating kinetic energy associated with fluctuations in single-phase flow and gas-solid two-phase flow are very different. In the former the energy flow is predominant from large scale to small scale, while in the latter it is more complicated. Clusters form initially at small length and time scales, and will grow into larger scales. The fluctuation energy is dissipated by collisions of particles and so there is almost certainly some energy flow from the very small scale to larger scales.

A cluster structure-dependent (CSD) drag coefficient model was proposed by Shuai et al. [25,26] on the basis of the minimization of energy dissipation by heterogeneous drag (MEDHD). In the CSD drag model, gas and particles are considered to be either in the particle-rich dense phase or in the gas-rich dilute phase. This means that in a grid cell particle movement is in the form of clusters in the dense phase or in the form of a dispersed particle in the dilute phase. Eight inhomogeneous structure variables ($U_{g,den}$, $U_{s,den}$, $U_{g,dil}$, $U_{s,dil}$, ε_{dil}, ε_{den}, f and d_c) with two dependent parameters ($a_{s,dil}$ and $a_{s,den}$) are solved by means of seven equations and a stability condition (minimization of energy dissipation by heterogeneous drag) to close the CSD drag model. In this original CSD drag model, the cluster diameter d_c proposed by Li et al. [11] in the EMMS drag model was used. This equation of cluster diameter d_c is assumed to be inversely proportional to the energy used for the suspension and transportation and by imposing two constraints, i.e. (1) its value approaches to infinity at the minimum fluidization and (2) to particle diameter at the maximum voidage. The derivations are on the basis of Chavan and Mashelkar method [27], and it is only valid in the co-current upward gas-particle two-phase flow. To remedy this limitation in the original CSD drag model [25,26], in the present work a modified CSD drag model is proposed using the bivariate extreme value theory instead of equation of cluster diameter. The drag coefficient is calculated from eight independent variables ($U_{g,den}$, $U_{s,den}$, $U_{g,dil}$, $U_{s,dil}$, ε_{dil}, ε_{den}, f and d_c) and four dependent parameters ($a_{g,den}$, $a_{g,dil}$, $a_{s,den}$ and $a_{s,dil}$) by means of a micro-meso-grid scales (M2GS) equation set which consists of six equations and the minimum energy dissipation by heterogeneous drag forces as a stability criterion with bivariate extreme value (BEV) theory. The relation between the modified CSD drag coefficient and the meso-scale structure variables is investigated. The modified CSD drag model is incorporated into the two-fluid model combining with kinetic theory of granular flow. The flow behavior in the gas–solid riser is simulated and compared with experimental results published in the literature.

2. Gas–solid two-fluid model with modified CSD drag model

In the present work, an Eulerian multi-fluid model, which considers the conservation of mass and momentum for the solid and gas phases, has been adopted. The kinetic theory of granular flow, which considers the conservation of solid fluctuation energy, has been used for closure. The governing equations are given below.

2.1. Governing equations

For simplicity, the following hypotheses are considered: (1) both gas phase and solid phase are assumed to be isothermal without chemical reactions. (2) the solid phase is characterized by a mean particle diameter and density. Both phases are continuous assuming a single gas phase and a single solid phase. The governing equations for each phase and the constitutive relations are given in Table 1 [5,25,26]. The continuity for gas phase and solid phase is expressed by Eq. (T1-1) and (T1-2). Mass exchanges between the phases are not considered because of no chemical reactions.

The momentum balance for the gas phase is given by the Navier–Stokes equation, modified to include an interphase momentum transfer