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CFD simulation of bubbling fluidized beds using a local-structure-dependent drag model

Jiageng Li, Bolun Yang *

Department of Chemical Engineering, State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University, Xi'an, Shaanxi 710049, PR China

HIGHLIGHTS

- The local-structure-dependent drag model based on a computational cell is established.
- A computational cell is resolved into three sub-systems.
- The meso-scale structural parameters and drag force are correlated by implementing the scale resolution.
- The grid independence of the new drag model is tested.
- The prediction accuracy of the new drag model is significantly improved compared with Gidaspow model.

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ABSTRACT

Conventional drag models coupled with a two-fluid model (TFM) are subject to certain restrictions on the predictions of the hydrodynamic behaviors in bubbling fluidized beds with fine particles, owing to the lack of scale resolution and the subsequent neglect of the impact of the meso-scale structure on gas-solid interaction. In this work, a local control volume is resolved into three sub-systems (i.e., the emulsion phase, bubble phase, and interphase) by implementing a designed route of scale resolution. Then, a local-structure-dependent (LSD) drag model based on the energy-minimization multi-scale (EMMS) theory is developed to account for the dependence of the drag force on the meso-scale structure. The LSD drag model is solved using a genetic algorithm and the obtained heterogeneous drag forces are integrated with the TFM to simulate the hydrodynamic behaviors in bubbling fluidized beds for different gas-solid systems. Consequently, the proposed drag model is validated to provide satisfying predictions of the fluidizations of Geldart A, A/B, and B particles. Furthermore, bubble diameters obtained from computational fluid dynamics (CFD) simulations are compared with those obtained from the empirical or semi-empirical correlations. The results indicate that the LSD drag model can capture the gas-solid hydrodynamics in a bubbling fluidized bed.

1. Introduction

Gas-solid fluidization processes taking place in bubbling fluidized bed reactors provide a considerable gas-solid interface area, which enhances the mass transfer significantly. Meanwhile, owing to the large heat capacity of the particles and the frequent contacts of gas to particles and particles to wall, the dense region of a fluidized bed reactor is nearly isothermal and the hotspot temperature is considerably smaller than that of the gas-solid fixed bed. The aforementioned advantages of a fluidized bed are favorable for numerous industrial processes involving mass and heat transfer, in particular for highly exothermic gas-solid catalytic reactions, such as methanation from synthesis gas or lignocellulosic biomass [1–3]. However, the phenomena of bubbling and elutriation become more significant in the scale-up of a bubbling fluidized bed [4]. This is attributed to: a) too large bubbles may reduce the gas-solid contact area and then diminish the mass transfer coefficient; and b) the elutriation due to the high gas velocity probably results in the loss of valuable reactants or catalyst particles [4,5]. As a result of these negative effects, the scale-up of a bubbling fluidized bed remains a complex and challenging endeavor [5].

With the rapid development of high-performance computers and numerical techniques, computational fluid dynamics (CFD) simulation is a promising tool to prevent the undesirable scale-up effects of a bubbling fluidized bed [5–7]. The CFD simulation has the potential to predict the entire process, including momentum transfer, mass transfer, heat transfer, and chemical reactions

* Corresponding author.
E-mail address: blunyang@mail.xjtu.edu.cn (B. Yang).

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Nomenclature

A area of a bubble occupied in the contours of transient solid volume fraction (m^2)
a_b acceleration of virtual particles in the interphase ($m \cdot s^{-2}$)
$a_{b,single}$ acceleration of a single virtual particle in the interphase ($m \cdot s^{-2}$)
a_{pb} acceleration of particles in the bubble phase ($m \cdot s^{-2}$)
$a_{pb,single}$ acceleration of a single particle in the bubble phase ($m \cdot s^{-2}$)
a_{pe} acceleration of a particles in the emulsion phase ($m \cdot s^{-2}$)
$a_{pe,single}$ acceleration of a single particle in the emulsion phase ($m \cdot s^{-2}$)
C_{D0} drag coefficient of a single particle (dimensionless)
C_{Db} drag coefficient of particle group in the bubble phase (dimensionless)
$C_{Db,0}$ drag coefficient of single particle in the bubble phase (dimensionless)
C_{De} drag coefficient of particle group in the emulsion phase (dimensionless)
$C_{De,0}$ drag coefficient of a single particle in the emulsion phase (dimensionless)
C_{Di} drag coefficient of virtual particle group in the interphase (dimensionless)
$C_{Di,0}$ drag coefficient of a single virtual particle in the interphase (dimensionless)
d_b bubble diameter or virtual particle diameter (m)
$d_{b,\max}$ maximum bubble diameter (m)
d_p particle diameter (m)
$f_{buoyancy,pb}$ buoyancy exerted on a single particle in the bubble phase (N)
$f_{buoyancy,pe}$ buoyancy exerted on a single particle in the emulsion phase (N)
$f_{buoyancy,(e\text{-}b)}$ buoyancy exerted on a single virtual particle in the interphase (N)
$F_{drag,b}$ drag force of the bubble phase per unit volume of bubble phase ($N \cdot m^{-3}$)
$F_{drag,e}$ drag force of the emulsion phase per unit volume of emulsion phase ($N \cdot m^{-3}$)
$F_{drag,i}$ drag force of the interphase per unit total volume ($N \cdot m^{-3}$)
$f_{drag,pb}$ drag force exerted on a single particle in the bubble phase (N)
$f_{drag,pe}$ drag force exerted on a single particle in the emulsion phase (N)
$f_{drag,(e\text{-}b)}$ drag force exerted on a single virtual particle in the interphase (N)
g gravitational acceleration ($m \cdot s^{-2}$)
H_d heterogeneity index (dimensionless)
$H_{\exp}$ bed expansion height (m)
m_{pb} mass of a single particle in the bubble phase (kg)
m_{pe} mass of a single particle in the emulsion phase (kg)
$m_{(e\text{-}b)}$ mass of a single virtual particle in the interphase (kg)
n_b number of particles in the bubble phase per unit volume of bubble phase (m^{-3})
n_e number of particles in the emulsion phase per unit volume of emulsion phase (m^{-3})
n_i number of virtual particles in the interphase per unit total volume (m^{-3})
N_s suspension energy consumption rates ($J \cdot s^{-1} \cdot kg^{-1}$)
$\Delta p/\Delta h$ pressure gradient ($Pa \cdot m^{-1} = N \cdot m^{-3}$)
Re_b particle Reynolds number in the bubble phase (dimensionless)
Re_e particle Reynolds number in the emulsion phase (dimensionless)
Re_i particle Reynolds number in the interphase (dimensionless)
Re_p particle Reynolds number in a control volume (dimensionless)
U_c transition velocity from a bubbling fluidized bed to a turbulent bed ($m \cdot s^{-1}$)
u_g superficial gas velocity in a control volume ($m \cdot s^{-1}$)
u_{gb} superficial gas velocity in the bubble phase ($m \cdot s^{-1}$)
u_{ge} superficial gas velocity in the emulsion phase ($m \cdot s^{-1}$)
u_p superficial particle velocity in a control volume ($m \cdot s^{-1}$)
u_{pb} superficial particle velocity in the bubble phase ($m \cdot s^{-1}$)
u_{pe} superficial particle velocity in the emulsion phase ($m \cdot s^{-1}$)
u_{slip} superficial slip velocity in a control volume ($m \cdot s^{-1}$)
$u_{slip,b}$ superficial slip velocity in the bubble phase ($m \cdot s^{-1}$)
$u_{slip,e}$ superficial slip velocity in the emulsion phase ($m \cdot s^{-1}$)
$u_{slip,i}$ superficial slip velocity in the interphase ($m \cdot s^{-1}$)
V_b virtual particle volume in the interphase (m^3)
V_{pb} particle volume in the bubble phase (m^3)
V_{pe} particle volume in the emulsion phase (m^3)
V_{total} total volume of control volume

Greek symbols
β_E heterogeneous drag coefficient ($kg \cdot m^{-3} \cdot s^{-1}$)
$\beta_{\text{Wen and Yu}}$ drag coefficient obtained from Wen and Yu drag model ($kg \cdot m^{-3} \cdot s^{-1}$)
δ_b bubble volume fraction (dimensionless)
ε_b voidage of the bubble phase (dimensionless)
ε_e voidage of the emulsion phase (dimensionless)
ε_g voidage of a control volume (dimensionless)
$\varepsilon_{g,L}$ lower bound of local voidage (dimensionless)
$\varepsilon_{g,U}$ upper bound of local voidage (dimensionless)
ε_{mf} minimum fluidization voidage (dimensionless)
μ_e viscosity of the emulsion phase ($Pa \cdot s$)
μ_g gas viscosity ($Pa \cdot s$)
ρ_b density of the bubble phase ($kg \cdot m^{-3}$)
ρ_e density of the emulsion phase ($kg \cdot m^{-3}$)
ρ_g gas density ($kg \cdot m^{-3}$)
ρ_p particle density ($kg \cdot m^{-3}$)

in a bubbling fluidized bed reactor. Of these transfer processes and reactions, the gas-solid momentum transfer is the most fundamental to reveal the entire processes. Nevertheless, multiphase flow in a bubbling fluidized bed is fairly complex owning to its inherent characteristic of nonlinearity and imbalance. Therefore, there remain quite a few challenges in its CFD simulation [8,9]. There are three main categories of CFD models for the simulation of the gas-solid flow in a fluidized bed: discrete-particle models (DPM), pseudo-particle models (PPM), and two-fluid model (TFM) [10]. The DPM is an Eulerian-Lagrangian approach in which gas is treated as a continuous phase and particles are treated as a discrete phase. Thus, the movement of gas phase can be obtained by solving the Navier-Stokes equations; the trajectory of a discrete particle is predicted by Newton's second law. To simulate the dense gas-solid flow in a bubbling fluidized bed, the particle-particle interactions cannot be neglected; thus, it demands considerable computational resources to track all of the particles when taking account of their interactions. The PPM is a pure Lagrangian approach in which gas