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Original Research Paper

Effect of drag models on CFD–DEM predictions of bubbling fluidized beds with Geldart D particles

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ABSTRACT

The selection of a drag model is of critical importance for fluidized bed simulations. In this study, the effect of different drag models was investigated by conducting Computational Fluid Dynamics and Discrete Element Method (CFD–DEM) simulations of bubbling fluidized beds and comparing the results with two sets of experimental data. For the data reported by Goldschmidt et al. (2004), the Di Felice model resulted in average particle height with less than 16% discrepancy, while the other drag models resulted in significantly lower values with discrepancies between 11 and 45%. For the NETL data (Gopalan et al., 2016), all the drag models showed reasonable qualitative agreement for the radial profiles of the solid velocities; however, no single model resulted in close quantitative predictions. None of the models were found to be suitable for both data sets. The analysis suggests that the Ayeni model and Di Felice model provide better predictions than the conventionally used Gidaspow model and Syamlal–O'Brien model.

1. Introduction

Bubbling fluidized beds (BFBs) are used in many industrial processes, including combustion, polymerization, pyrolysis, and catalytic cracking. In a BFB, gas–solid hydrodynamics govern the mixing between the two phases and thus its performance. As a result, the flow inside a BFB has been extensively studied both experimentally and using computational fluid dynamics (CFD). The available gas–solid flow models can be broadly divided into two categories: Eulerian–Eulerian (EE) or Eulerian–Lagrangian (EL). In the EL models, also known as discrete particle models (DPM), the gas phase is assumed to be continuous and the solid phase is treated as discrete particles. The EL models can be further classified as unresolved-DPM (u-DPM) and resolved-DPM (r-DPM) models based on the spatial discretization of the continuous phase [1]. In u-DPM models, the size of the Eulerian grid is larger than the size of the solid particles, whereas in r-DPM models, it is smaller than the solid particles. The u-DPM model is also referred to as a CFD–discrete element model (CFD–DEM). Simulations using CFD–DEM are computationally less intensive; hence, there has been growing interest in using them to investigate the hydrodynamics of BFBs.

In CFD–DEM, the flow of solids is resolved by solving the force balance equation, which includes the gravity, drag, contact, and other forces around each discrete particle. The drag represents the interphase exchange force between the gas and solids, and modeling it accurately is vital for reliable predictions [2–4]. Several drag models have been proposed in the literature, which can be classified into five categories: (i) those derived from the pressure drop in packed bed experiments (Ergun [5], Gibilaro [6,7] and Ayeni [3]), (ii) those obtained by correcting single particle drag models using settling experiments (Wen-Yu [8], Di Felice [9] and Syamlal–O'Brien [10]), (iii) hybrid models (Gidaspow [11]), (iv) multi-scale models (e.g., energy minimization multi-scale (EMMS) [12] and sub-grid scale filter [13–15], and (v) those derived from direct numerical simulations (Hill–Koch–Ladd (HKL) [16,17], Beetstra–van der Hoef–Kuiper (BVK) [18] and Tenneti et al. [19,20]). These models differ in their derivation method and applicability to different types of gas–solid flows.

As a result, many CFD studies have been conducted to investigate the effect of drag models on flow predictions [2–4,21–31]. Most of these studies have used EE models, while a few studies have employed the CFD–DEM model (Li and Kuipers [21], Ku et al. [2], Ayeni et al. [3], Koralkar and Bose [4], Di Renzo et al.

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Nomenclature

a	tuning parameter of Syamlal–O'Brien drag model (–)
A_p	projected surface area of a particle (m^2)
b	tuning parameter of Syamlal–O'Brien drag model (–)
CF	correction factor (–)
$C_{D,H}$	drag coefficient for a single particle in a multi-particle system (–)
$C_{D,\infty}$	drag coefficient for a single isolated particle in an infinite domain (–)
d_p	diameter of a particle (m)
$\overline{\overline{D_G}}$	strain rate tensor (s^{-1})
e	coefficient of restitution (–)
$\boldsymbol{f}_D$	drag force on a single isolated particle in an infinite domain (kg·m/s^2)
$\boldsymbol{f}_{D,H}$	drag force on a single particle in a multi-particle system (kg·m/s^2)
$\boldsymbol{F}_C^{(i)}$	net contact force as a result of contact with another particle (kg·m/s^2)
$\boldsymbol{F}_D$	total drag force on all particles in a unit control volume (kg·m/s^2)
$\boldsymbol{F}_d^{(ij)}$	dashpot force between the i^{th} and j^{th} particles (kg·m/s^2)
$\boldsymbol{F}_s^{(ij)}$	spring force between the i^{th} and j^{th} particles (kg·m/s^2)
$\boldsymbol{F}_T^{(i)}$	net sum of all forces acting on the i^{th} particle (kg·m/s^2)
$\boldsymbol{g}$	acceleration due to gravity (m/s^2)
$h^{(i)}$	axial height of the i^{th} particle (m)
$\langle h_p \rangle_{bed}$	average particle height (m)
$I^{(i)}$	moment of inertia of the i^{th} particle (kg·m^2)
$\boldsymbol{I}_{GS}$	momentum transfer between gas and solid phases (kg/m^2·s^2)
k	spring stiffness coefficient (kg/s^2)
$L^{(i)}$	distance of the contact point from the center of the i^{th} particle (m)
$m^{(i)}$	mass of the i^{th} particle (kg)
m_{eff}	effective mass (kg)
N_p	number of particles (–)
P_G	gas phase pressure (kg/m·s^2)
Re_P	particle Reynolds number (–)
$\overline{\overline{S_G}}$	gas phase stress tensor (kg/m·s^2)
t_n^{col}	collision time between two particles (s)
$\boldsymbol{t}^{(ij)}$	tangent to the plane of contact between the i^{th} and j^{th} particles
$\boldsymbol{T}^{(i)}$	sum of all torques acting on the i^{th} particle (kg·m^2/s^2)
$\boldsymbol{u}$	local linear velocity (m/s)
$\boldsymbol{U}_G$	inlet gas velocity (m/s)
$\boldsymbol{U}_{mf}$	minimum fluidization gas velocity (m/s)
U_{slip}	slip velocity (m/s)
V_p	volume of a single particle (m^3)
$\boldsymbol{X}$	particle location (–)
x, y, z	x, y and z direction in Cartesian coordinate system (Fig. 2)

Subscripts

C	contact force
d	dashpot
D	drag force
G	gaseous phase
Gidaspow	Gidaspow drag model
H	hindered flow condition
mf	minimum fluidization condition
n	properties in normal direction
p	solid particle
s	spring
S	solid phase
t	properties in tangential direction

Superscripts

i	i^{th} particle
j	j^{th} particle
ij	i^{th} and j^{th} particle pair
k	k^{th} cell
$i \in k$	i^{th} particle residing in k^{th} cell

Greek letters

β	gas - solid momentum exchange coefficient (kg/s)
δ_n	normal overlap between particles (m)
δ_t	tangential displacement (m)
ϵ	volume fraction (–)
$\eta^{(ij)}$	unit vector along the line of contact pointing from particle i to particle j (–)
η	damping coefficient (kg/s)
λ_G	second coefficient of viscosity of the gas phase (kg/m·s)
μ_G	dynamic viscosity of gas (kg/m·s)
ν	coefficient of friction (–)
$\omega^{(i)}$	angular velocity of the i^{th} particle (rad/s)
ρ	density (kg/m^3)
$\overline{\overline{\tau_G}}$	gas phase shear stress tensor (kg/m·s^2)
θ	granular temperature (m^2/s^2)
$\vartheta^{(k)}$	volume of k^{th} cell (m^3)

Abbreviations

2D	two dimensional
BFB	bubbling fluidized bed
BVK	Beetstra–van der Hoef–Kuipers
CF	correction factor
CFD	computational fluid dynamics
DPM	discrete particle model
DEM	discrete element model
EE	Eulerian–Eulerian
EL	Eulerian–Lagrangian
EMMS	energy minimization multi-scale
GenIDLEST	generalized incompressible direct and large eddy simulation of turbulence
HKL	Hill–Koch–Ladd
MFiX–DEM	Multiphase Flow with interphase eXchange–Discrete Element Model
NETL	National Energy Technology Laboratory

[32] and Zhang et al. [33]). Furthermore, the majority of previous studies were conducted for either Geldart A or B particles. Only Ayeni et al. [3], Koralkar and Bose [4] and Ku et al. [2] have investigated the effect of drag models on CFD–DEM simulations of BFBs with Geldart D particles. The fluidization of different Geldart particles types manifests different behaviors [34–39] owing to the different relative magnitudes of inter-particle cohesive forces and interphase interactions in the bed [36]. Thus, simulation of particles from a particular Geldart group requires selection of an appropriate drag model. Ku et al. [2] assessed the Gidaspow, Di Felice, and HKL models, and concluded that their predictions for the pressure drop and its fluctuations agreed with each other. They observed that the Gidaspow model resulted in the lowest fluctuation frequency, whereas the Di Felice model resulted in

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