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Simulation of 3D freely bubbling gas–solid fluidized beds using various drag models: TFM approach

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ABSTRACT

In this article, 3D modeling and simulation of bubbling fluidized beds has been conducted using various drag models, and the model predictions were validated against reported experimental data and 2D simulation results. In this regard, different drag models reported in the literature including Gidaspow, Syamlal–O'Brien, Hill–Koch–Ladd, and Wen–Yu were applied. A standard Two-Fluid Model (TFM) closed by the Kinetic Theory of Granular Flows (KTGF) was used to simulate bubbling gas–solid fluidized beds. Excellent agreements between the simulation results and experimental data, concerning bed expansion ratio, gas volume fraction, and time-averaged particles velocity, were found over a wide range of particle size, static bed height, and fluidization velocity. Moreover, comparison of 2D and 3D simulation results with experimental data shows that overpredictions attributed to 2D simulations can be a direct result of neglecting frictional stresses. In addition, it was found that the Wen–Yu drag model can provide better predictions for the bed expansion ratio and solids velocity relative to other drag models.

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1. Introduction

Gas–solid fluidized beds, as one of the most important contacting devices, have been widely used in chemical and petroleum industries owing to their excellent gas–solid contact and favorable heat- and mass-transfer characteristics. Undoubtedly, the presence of gas bubbles in fluidized beds contributes both to their beneficial characteristics as well as their undeniable limitations and drawbacks. Considerable efforts have, therefore, been devoted to understand the formation and behavior of gas bubbles in fluidized beds. In this regard, two-dimensional fluidized beds, in planar rectangular columns of very limited thickness, have been often used to investigate the fundamental basis of fluidization such as bubble specifications, flow patterns, and solids mixing (Busciglio et al., 2008, 2009; Caicedo et al., 2003; Soler et al., 2003; Pallares and Johnsson, 2006; Shen et al., 2004; Lim et al., 2007).

In recent years, computational fluid dynamics (CFD) has been frequently employed as a strong tool to investigate the

inherent complex hydrodynamics of fluidized beds. However, it should be noted that in the development and application of CFD, careful validation against experimental data is always required (Grace and Taghipour, 2004). Accordingly, extensive experimental investigations on two-dimensional fluidized beds can be appropriately used to explore the validity of the numerical simulations. However, most simulations have been conducted in a simple two-dimensional configuration by ignoring the front and back walls of the experimental columns (Busciglio et al., 2009; Taghipour et al., 2005). Although it might be clear that the walls would significantly affect the hydrodynamics of the thin fluidized beds, little attention has been paid to the wall effect in numerical simulations of pseudo-two-dimensional fluidized beds.

Almost for sure, two-fluid model (TFM) whereby both the fluid and solid phases are treated as interpenetrating continuum phases is the most commonly used approach for the simulation of fluidized beds (Pain et al., 2001). In this approach, particle phase would be mathematically modeled

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Nomenclature

C_D	drag coefficient (dimensionless)
$D_{g,ij}$	rate of strain tensor for fluid phase (s^{-1})
d_p	particle diameter (m)
D_{sij}	rate of strain tensor for solid phase, (s^{-1})
e	restitution coefficient (dimensionless)
\bar{g}	gravitational acceleration ($m s^{-2}$)
$g_{0,ss}$	solid radial distribution function
H_0	static bed height (m)
\bar{I}	identity matrix
I_{2Dg}	second invariant of the deviator of the strain rate tensor for gas phase (s^{-2})
I_{2Ds}	second invariant of the deviator of the strain rate tensor for solid phase (s^{-2})
I_{gs}	interaction force between gas and solid phases ($kg m^{-2} s^{-2}$)
J_s	rate of pseudo-thermal energy dissipation due to inelastic collisions ($m^2 s^{-3}$)
l_s	a turbulence length-scale parameter (m)
\hat{n}	unit normal vector from the boundary into the particle assembly
P	pressure (Pa)
P_c	critical state solid frictional pressure (Pa)
q	diffusive flux of pseudo-thermal energy ($kg s^{-3}$)
Re	Reynolds number (dimensionless)
t	time (s)
V_{Ts}	ratio of terminal velocity of multiparticle and single particle (dimensionless)

Greek symbols

β_{gs}	gas–solid momentum exchange coefficient ($kg m^{-3} s^{-1}$)
ε	volume fraction (dimensionless)
ε^*	bed voidage at minimum fluidization conditions (dimensionless)
$\varepsilon_{s,max}$	maximum packing limit (dimensionless)
Θ	granular temperature ($m^2 s^{-2}$)
κ	solid thermal conductivity ($kg m^{-1} s^{-1}$)
$\kappa_{\Theta s}$	diffusion coefficient of granular energy ($kg m^{-1} s^{-1}$)
μ	solid phase granular viscosity (Pa s)
μ_b	solid phase bulk viscosity (Pa s)
μ_e	solid phase eddy viscosity (Pa s)
μ_f	solid phase frictional viscosity (Pa s)
μ_{gt}	solid phase turbulent viscosity (Pa s)
μ_s	solid phase shear viscosity (Pa s)
\vec{v}	local velocity ($m s^{-1}$)
\vec{v}_{mf}	superficial gas velocity at minimum fluidization conditions ($m s^{-1}$)
$\vec{v}_{sl, }$	slip velocity of particle assembly at the wall ($m s^{-1}$)
ξ	specularity coefficient (dimensionless)
Π_s	net rate of pseudo-thermal energy dissipation due to gas–particle interactions ($kg m^{-1} s^{-3}$)
ρ	density ($kg m^{-3}$)
τ	stress tensor ($kg m^{-1} s^{-2}$)
ϕ	angle of internal friction (deg)
∇	gradient operator (m^{-1})

Subscripts/superscripts

b	bulk
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exp	experiment
f	frictional
g	gas phase
max	maximum
mf	minimum fluidization
min	minimum
p	particle phase
pp	particle–particle
s	solid phase
sim	simulation
sw	solid–wall
T	transpose
w	wall

using well-known continuum mechanics. The solid particles are generally considered to be identical and have a representative diameter and density. The main principle of TFM is to treat each phase as an interpenetrating continuum to setup integral balances of continuity, momentum, and thermal energy for both the phases along with imposing appropriate boundary conditions and jump conditions at the interface. Since the resultant continuum approximation of the solid phase has no equation of state and lacks a number of predominant parameters such as viscosity and normal stress (Pain et al., 2001), certain averaging techniques and assumptions are required to derive momentum balance equations for this phase.

Numerous improvements have been developed to simulate bubbling gas–solid fluidized beds using TFM approach. In recent years, mass conservation and momentum balance for gas and solid phases were applied to simulate the hydrodynamics of bubbling gas–solid fluidized beds. By analogy with the use of the kinetic theory of gases, the kinetic theory of granular flows (KTGF) was introduced into TFM to improve the description of particles collision (Chapman and Cowling, 1970). Hence, the kinetic theory of granular flows has been numerous employed by investigators who participated in the modeling and simulation of gas–solid flows in fluidized beds and risers. Moreover, it has been found that the KTGF has a certain advantage in the perfect predictions of flow phenomena for the systems with dilute and dense phases (Arastoopour, 2001; Bi et al., 2000; Gidaspow, 1994).

The kinetic theory of granular flows as well as the closure models are derived assuming that the particles have the same diameter (i.e., mono-disperse suspensions). This is while in most engineering applications, we deal with polydisperse suspensions, which mean that the suspension consists of particles with different diameters and densities. In a system consisting of particles of identical density, but different sizes, the bigger (heavier) ones tend to reside at the bottom of the bed and the smaller (lighter) ones show the tendency to float and reside at the bed surface. Employing the kinetic theory of granular flows for the theoretical descriptions of suspensions with more than one particle size, was developed and reformulated by Jenkins and Mancini (1989). They predicted the transport properties of a binary mixture of smooth and slightly inelastic spheres. Furthermore, in their study, the granular temperature of the included particles was corresponded to the kinetic energy of a binary mixture.

Zamankhan (1995) developed a kinetic theory for a binary mixture of spherical particles involving perturbations to the Maxwellian velocity distribution as well as assumed that the

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