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Impacts of solid-phase wall boundary condition on CFD simulation of conical spouted beds containing heavy zirconia particles

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ABSTRACT

The gas–solid flow behavior of a conical spouted bed including heavy particles, zirconia, with density of 6050 kg/m^3 that typically encountered in chemical vapor deposition (CVD) was studied by the CFD technique. An Eulerian–Eulerian two-fluid model (TFM) in conjunction with the kinetic theory of granular flows (KTGF) was used in a full 3D computational framework. To reduce the computational time, while maintaining the accuracy of the results, polyhedral mesh structure was utilized. Parametric studies of the specularity coefficient and particle–wall restitution coefficient were also performed. The hydrodynamics parameters including particle velocity and solid volume fraction profiles at different bed levels were evaluated, and the overall behavior of particles in the bed was studied. The simulation results showed that the specularity coefficient significantly affects the CFD results, while the impact of small changes in the particle–wall restitution coefficient is not noticeable. Furthermore, a small specularity coefficient of 0.05 provides suitable predictions that are in agreement of the experimental data. Incoherent spouting was also properly predicted by the present CFD model, which was shown to be in agreement with the experimental observations. It was also found that both the no-slip boundary condition and the specularity of $\varphi = 1$ wall boundary condition predict roughly the same results. Finally, the influences of the drag function and particle–particle restitution coefficient on the CFD results were studied, and the new findings were discussed.

1. Introduction

The spouted beds are widely used in various industrial applications such as the drying of grains, spray drying, coating, heterogeneous catalysis, and gasification of biomass and coal. In coating aspect, for instance, TRISO (tri-structural-isotropic) nuclear fuel structure is based on coated kernels of discrete UO_2 or UCO particles. These coaters are carbon and silicon carbide layers that are added to the kernels by chemical vapor deposition (CVD) in the conical spouted bed reactors at high temperatures. Detailed hydrodynamics of conical spouted bed reactors are necessary for design, scale-up, and developing a fabrication process of these fuel coaters. Modeling of hydrodynamics of fuel coaters that controls how the fuel particles and reactant gases are mixed and heated is important for improving the efficiency of the process. In addition, the CFD simulations provide information on temporal changes that cannot be obtained experimentally and yet useful for design of the reactor. In the recent years, computational fluid dynamics (CFD) has emerged as an effective tool for predicting the behavior of gas–solid flows. This is the consequence of rapid increase of computational hardware capacity, together with the recent advances in numerical algorithms, and deeper understanding of physics of multiphase flows.

Previous studies that are entirely limited to the relatively light particles ($\rho < 3000$ kg/m^3) have shown that the particle density significantly affects the hydrodynamic behavior [1,2]. In addition, Zhou and Bruns [3] found that different correlations from the literature, which have driven for the lower density particles in spouted beds, predict the results with the highest deviation from the experimental measurements of heavy particles of ZrO2. They also developed a new minimum spouting correlation for shallow conical spouted beds including heavy particles.

The hydrodynamics of the spouted beds containing light particles (with densities around 3000 kg/m^3 or less) are extensively studied by a number of researchers [4–8]. However, only

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Nomenclature

C_D	drag coefficient [–]
d_s	particle diameter [m]
D_s	diameter of the spout gas inlet [m]
D_t	diameter of the bed [m]
H	vessel height [m]
e_s	particle–particle restitution coefficient [–]
e_w	particle–wall restitution coefficient [–]
g	acceleration due to gravity [m/s^2]
g_0	radial distribution coefficient [–]
H_0	static bed depth [mm]
$\bar{I}$	stress tensor [–]
I_{2D}	second invariant of the deviatoric stress tensor [–]
$k_{\Theta s}$	diffusion coefficient for granular energy [kg/m s]
β	gas–solid momentum exchange coefficient [kg/m^3 s]
β_{Ergun}	gas–solid momentum exchange coefficient by Ergun equation [kg/m^3 s]
$\beta_{Wen\text{-}Yu}$	gas–solid momentum exchange coefficient calculated by Wen-Yu equation [kg/m^3 s]
P	pressure [N/m^2]
P_s	solids pressure [N/m^2]
t	time [s]
U	superficial gas velocity [m/s]
v_i	velocity [m/s]

Greek letters

α_i	volume fraction [–]
γ_s	the collisional dissipation of energy [kg/s^3 m]
Θ_s	granular temperature [m^2/s^2]
λ_s	solid bulk viscosity [kg/m s]
μ_i	shear viscosity [kg/m s]
ρ_i	density [kg/m^3]
$\bar{\bar{\tau}}_i$	stress tensor [N/m^2]
ϕ	angle of internal friction [degree]
φ	specularity coefficient [–]

Subscripts

col	collision
fr	friction
kin	kinetic
g	gas
p	particle
q	phase type (solid or gas)
s	solids
T	stress tensor

few studies have been reported in the literature regarding the hydrodynamics of conical spouted beds including the heavy particles with densities of the order of 6000 kg/m^3, which occur in the nuclear fuel particles coating process [9–12]. In particular, Pannala et al. [9] studied a 2D conical spouted bed containing heavy zirconia particles (6000 kg/m^3) using the MFIX code, where they observed incoherent spouting in the bed. More recently, Lüle et al. [12] performed a 2D CFD simulation of a conical spouted bed containing zirconia particles and investigated the effects of bed geometric such as conical angle and static bed height, as well as, the operational factors.

Consequently, further detailed investigations are required to delineate the systems operating with heavy particles.

Several CFD studies of various types of spouted beds containing light particles such as conical–cylindrical spouted beds [4], conical–cylindrical spouted beds with draft tube [13,14] and pseudo 2D spouted beds [5,15,16] were reported in the literature. In these simulations of spouted beds, no-slip, partial-slip and free-slip wall boundary condition for the solid phase were used. The no-slip boundary condition was most commonly used [17–27], while the particle-partial slip boundary condition was used by Bettega et al. [28]. The free-slip boundary condition was only used by Wang et al. [29].

For CFD simulations of gas–solid fluidization systems, it is well known that the use of suitable wall boundary conditions for gas and solid phases is critical for proper prediction of the hydrodynamics of these systems. This has to be further emphasized in [30] for the case of laboratory and small-scale fluidized bed columns. Some of the recent CFD studies of gas–solid systems that were focused on the impact of solid-wall boundary conditions are described in this section:

Zhang and Yu [31] showed that the slugging behavior of fluidized beds with Geldart B particles was greatly affected by the wall boundary conditions. Benyahia et al. [32] found that the specularity coefficient significantly affect the behavior of gas–solid flows for dilute as well as dense flow conditions where particles collisions are dominant. Benyahia et al. [33] also reported that the use of a low value of specularity coefficient led to proper prediction of the core-annulus flow regime in a vertical channel containing glass beads. Almuttahar and Taghipour [34] showed that using a small specularity coefficient for wall boundary condition for the flow of FCC particles in a dense circulating fluidized bed led to the reasonable results. They also reported that the changes in the particle–wall restitution coefficient, e_w, did not markedly affect the simulation results. Similar trends were found by Wang et al. [35] in their CFD study of hydrodynamics of a high flux circulating fluidized bed with Geldart group A particles. Li et al. [36] emphasized the importance of careful prescription of the solid-phase wall boundary condition for proper prediction of gas mixing in the bubbling fluidized bed including glass beads. Zhong et al. [37] studied the segregation and mixing of binary particle mixtures in 2D geometry and found that for low values of specularity coefficient ($\varphi = 0$, 0.0005), segregation did not occur. The mixing, however, was not influenced for a wide range of φ. Altantzis et al. [38] showed that for a thin rectangular fluidized bed, the choice of φ even alter the fluidization regime, for instance slug formation being characteristic for lower values of φ. More recently, Bakshi et al. [39] studied the impact of φ on the fluidization hydrodynamics for full 3D simulation in cylindrical coordinate. They suggested that values of φ in the range (0.01,0.3) were suitable for simulation of most dense gas–solid flows.

For CFD simulation of conical–cylindrical spouted beds, Lan et al. [8] examined the effects of specularity coefficient and particle–wall restitution coefficient and found that φ had a significant effect on the spouting behavior, while the model results is not influenced by small changes in the particle–wall restitution coefficient. Hydrodynamics of a conical–cylindrical spouted bed with a draft tube was studied by Hosseini et al. [13]. They showed that the model predictions for particle behavior through the draft tube are sensitive to the values of specularity and particle–wall restitution coefficients.

From the presented review of literature it appears that there is no consistency on the kind of wall boundary conditions that should be used for proper modeling of the interactions between the light particles and the wall. In this study the gas–solid flow behavior in a 3D conical spouted bed including heavy zirconia particles was studied using the two-fluid model (TFM) in conjunction with kinetic theory of granular flows (KTGF). The simulation results were compared with the corresponding experimental data of Lüle et al. [12]. It is imperative to note that the use of proper value of φ is important in simulations of gas–solid systems that are inherently 3D such as mixing and segregation. Accordingly, parametric studies of the effects of specularity coefficient and particle–wall