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EULER-EULER AND EULER-LAGRANGIAN EVALUATION OF A PSEUDO-2D GAS FLUIDIZED BED: AN ESTIMATION OF THE WALL BOUNDARY CONDITION FROM DEM

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ABSTRACT

In this work a new partial slip boundary condition for the solid phase in pseudo-2D beds is estimated from DEM simulations and implemented in a two-fluid model. The high spatial resolution of the DEM allowed us to obtain the information required for the new boundary condition, viz. the particle interaction with the walls. In addition, the new boundary condition is compared with the classical Johnson and Jackson boundary condition, which is commonly employed in two-fluid models. The variation of the parameters of the new boundary condition with the superficial gas velocity, and with the coefficients of restitution and friction for particle-particle and particle-wall contacts, is studied. The results show that the coefficient of friction is the most influential parameter in the wall boundary condition.

INTRODUCTION

Numerical modelling of fluidized beds has advanced significantly over the last decades; the most popular modelling approaches being the Eulerian-Eulerian and the Eulerian-Lagrangian models. In the development and application of these techniques, careful validation with either experimental data or theoretical models is required (1).

In a bed of small thickness, i.e. a pseudo two-dimensional (2D) bed, the front and the rear walls restrict the solids motion, leading to different flow behaviour compared to fully three-dimensional (3D) systems. For beds of small transverse thicknesses, the effect of the front and the rear walls on the particle motion can be significant and should not be neglected. Li et al. (2) investigated the influence of the particle wall boundary condition (BC) by performing 2D and 3D Eulerian-Eulerian simulations of a pseudo-2D fluidized bed and concluded that the wall effects play an important role in CFD simulations. Hernández-Jiménez et al. (3) studied a pseudo-2D fluidized bed using 2D Eulerian-Eulerian simulations and PIV measurements and reported that the 2D simulations systematically overpredict the solids velocity. It was argued that this discrepancy is caused because the effects of the front and rear walls on the particle motion was neglected. Besides, it is not clear whether general BCs for two-fluid models, which assume that the particles interact with a single surface are valid for pseudo-2D beds in which both the front and rear walls simultaneously affect the particle motion. More recently, Li and Benyahia (4) revisited the Johnson and Jackson (5) BC for granular flows, theoretically studying the collision between a particle and a flat wall. They suggested an analytical expression for the specularity coefficient, but also concluded that soft-sphere DEM simulations are needed properly to study the particle-wall interaction.

In this work a new partial slip BC for the solid phase in pseudo-2D beds is developed by means of DEM simulations and subsequently implemented in a two-fluid model. In the DEM the spatial resolution is sufficiently high to obtain information regarding the interaction of individual particles with the walls. The new BC is compared with the Johnson and Jackson BC (5), which is commonly employed in two-fluid simulations. The effect of the coefficients of restitution and friction for particle-particle and particle-wall contacts, as well as the effect of the superficial gas velocity on the parameter values of the newly proposed BC is studied.

NUMERICAL SIMULATIONS

The gas-fluidized bed studied was of width W = 0.15 m, height H = 0.2 m and thickness Z = 0.01 m, and was partially filled with spherical particles of density ρ_s = 2500 kg/m^3 and diameter d_p = 1.14 mm. The fluidizing gas was air and was uniformly injected through the base of the bed. The minimum fluidization velocity, U_{mf} , was 0.62 m/s. A fixed pressure BC was chosen at the top of the freeboard. The main simulation parameters are listed in Table 1. Several cases, varying the coefficient of restitution, the coefficient of friction between particles (which in DEM is the same as the coefficient of friction between particles and walls) and the gas velocity were studied and are summarized in Table 2. Case 1 was selected as the base case.

Parameter	**Value**
Particle density (kg/m^3)	2500
Gas density (kg/m^3)	1.2
Gas viscosity (Pa s)	1.8x10^{-5}
Particle diameter (mm)	1.14
Bed width (m)	0.15
Bed height (m)	0.2
Bed thickness (m)	0.01
Static bed height (m)	0.06

Table 1: Simulation parameters

Case	**U/U$_{mf}$**	**Coefficient of restitution (-)**	**Angle of internal friction (°)**
1	2	0.9	30
2	2	0.9	5.71
3	2	0.5	30
4	1.75	0.9	30
5	2.25	0.9	30

Table 2: Cases simulated using the DEM

A second order accurate scheme was used to discretize the convective derivatives for both modelling approaches. The 3D computational domain was discretized using cubic cells of length 3.3 mm. 55 seconds of physical time were used for time-averaging the simulation results of the solids velocity and concentration, and 25 seconds for the bubble diameter and velocity.

DEM approach

A Discrete Element Model (DEM) has been constructed based on the work of Tsuji et al. (6), which combines the discrete element model of Cundall and Strack (7) to simulate the particulate phase, with the volume-averaged Navier-Stokes equations for the fluid phase, as derived by Anderson and Jackson (8). To model collisions between contacting particles the soft-sphere approach was used, in which the particles are allowed to overlap by a small amount. In the direction normal to the particle surface a repulsive force between overlapping particles was modelled using a damped linear spring with a spring shiftness of 1000 N/m. In the tangential direction friction was modelled as a damped linear spring with a spring constant of 500 N/m and the magnitude of the force was limited by Coulomb's law. The fluid was assumed to be Newtonian. The number of particles simulated was 69611.

TFM approach

The two-fluid model (TFM), based on the conservation equations of mass, momentum and granular temperature, was solved using MFIX (Multiphase Flow with Interphase eXchanges) (Syamlal et al. (9) and Benyahia et al. (10)). The kinetic theory of granular flow was used for the closure of the solids stress terms. Details of the closure expressions used in MFIX can be found in Syamlal et al. (9). At the lateral walls partial slip was assumed for the solid phase. The initial solids volume fraction was set to 0.6.

In both modelling approaches (DEM and TFM) the drag force correlation proposed by Beetstra et al. (11) was employed to describe the momentum exchange between the gas and the solid phases.

RESULTS

Partial slip estimated from DEM

The shear force experienced by the bed particles at the wall is related to the gradient of their vertical velocity perpendicular to the wall, $\partial V_y/\partial Z$. As a first approximation, $\partial V_y/\partial Z$ is a function of the physical parameters of the bed (coefficient of restitution, e, coefficient of friction between particles, ϕ), the particle velocity at the wall, $V_{y,wall}$, the thickness of the bed, Z, and the solids concentration, α_s, which is calculated considering the volume of the particles in each cell. V_y is calculated making a simple arithmetic average of the particle velocities in a cell. Thus, dimensional analysis leads to:

$$\left.\frac{\partial V_y}{\partial Z}\right|_{wall} = g\left(e,\phi,V_{y,wall},Z,\alpha_s\right) \rightarrow \frac{Z}{V_{y,wall}}\left.\frac{\partial V_y}{\partial Z}\right|_{wall} = f(\alpha_s,e,\phi) \tag{1}$$

Using Equation 1, the spatial derivative of the particle vertical velocity can be expressed as a function of the vertical particle velocity at the wall:

$$\left.\frac{\partial V_y}{\partial Z}\right|_{wall} = h_w V_{y,wall} \tag{2}$$

where $h_w = f(\alpha_s,e,\phi)/Z$ is a partial slip coefficient, which depends on the solids concentration as well as the bed thickness and the coefficients of restitution and friction.

To estimate h_w the thickness of the bed was divided into 6 virtual cells and the two cells closest to a wall in the z-direction were used to estimate the particle velocity at the front and rear walls and the spatial derivative of the velocity at the walls of the bed. In each frame, the instantaneous velocity of the particles was spatially averaged in a cell of size 3.3x3.3x1.6 mm. Simulation data were recorded at 50 Hz for a time period of 10 s to perform this analysis. The cells near the distributor and near the bed surface were excluded from the analysis in order to avoid the effects of air injection and bubble eruption which may not be representative of the solids motion inside the bulk of the bed.

Figure 1 shows a set of scatter plots obtained from DEM simulations. Each point of the scatter plots represents a value of $\left(\partial V_y/\partial z\right)_{wall}$ versus $V_{y,wall}$ in a cell face at the bed wall. Each subfigure plots points within a certain range of α_s. Since the ranges of α_s are small, regression of a line in the scatter plots provides an estimation of the value of h_w in Equation 2 for a fixed α_s.

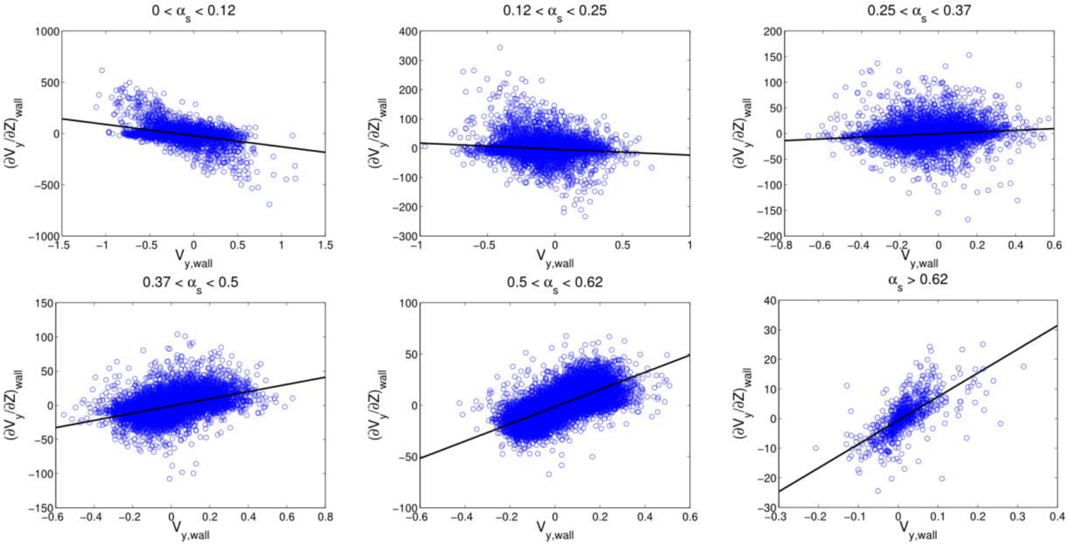

Figure 1: Spatial derivative of the particle velocity at the wall as a function of the velocity at the wall for different values of solids fraction, Case 1.

According to Figure 1, for values of the solids volume fraction larger than ~0.25, the regression lines in the scatter plots have a positive slope, as expected. However, for lower values of the solids volume fraction (α_s<0.25) the slopes of the regression lines are negative, which means that the magnitude of the vertical velocity increases close to the wall. This is opposite to the trend predicted by the Johnson and Jackson BC (5), which assumes that the effect of the wall is to retard particle motion. One possible explanation for this behaviour could be that in a quasi-2D bed particles interact with the gas flow and the walls in such a way that the faster particles tend to drift towards the walls when the solids volume fraction is small.

Using the slope of the lines in Figure 1, the values of the normalized partial slip coefficient $h_w Z = \left(\partial V_y/\partial z\right)_{wall}\left(Z/V_{y,wall}\right)$ can be plotted as a function of α_s. The best fit to this data was found to be of the form given by Eq 3.

$$\left(\frac{\partial V_y}{\partial Z}\right)_{wall}\left(\frac{Z}{V_{y,wall}}\right) = A\ln(\alpha_s) + B \tag{3}$$

Where *A* and *B* are obtained by fitting Eq. 3 to the slopes of the regression lines in Figure 1. Eq. 3 can be easily implemented in the TFM simulations as a partial slip

BC. Several attempts were made to study how other parameters affect this correlation, e.g. the granular temperature or the slip velocity. However none of these parameters were found to influence appreciably the functional form (Eq. 3) of the correlation proposed.

The results obtained for the new partial slip BC for quasi-2D beds, Eq. 3, are shown in Figure 2 together with the partial slip BC proposed by Johnson and Jackson (5) using the specularity coefficient $\phi = 0.005$, as recommended by Li et al. (2). The new partial slip condition follows a trend markedly different to that of the classical partial slip BC at low values of α_s. The negative value of the slope indicates that the magnitude of the particle velocity at the wall is typically greater than the velocity in the centre of the bed when the solids volume fraction is smaller than 0.25.

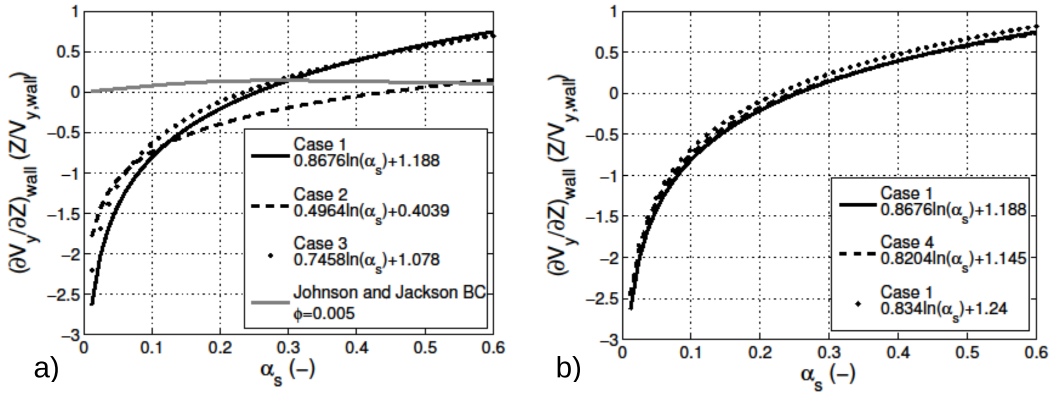

Figure 2: Logarithmic fit to the normalized partial slip coefficient versus the solids volume fraction: a) effect of the coefficients of restitution and friction and b) effect of the superficial gas velocity.

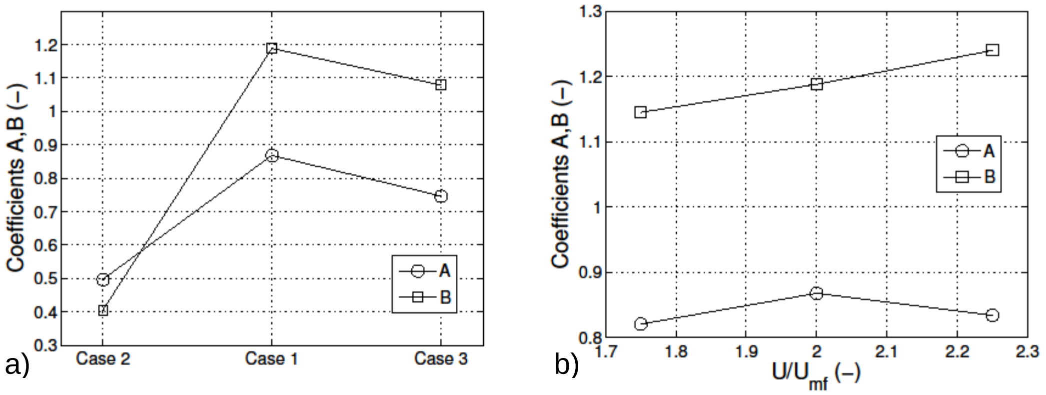

Figure 3: Coefficients *A* and *B* of Eq.3 obtained from the logarithmic fit shown in Figure 2.

Furthermore, it can be observed in Figure 2a that the coefficient of restitution has a smaller effect on the normalized partial slip coefficient than the coefficient of friction. The small friction coefficient used in Case 2 resulted in relatively small values of the partial slip coefficient for most solids concentrations. For this case the partial slip coefficient is only positive for high solids concentrations (0.5-0.6). Paying attention to the effect of the superficial gas velocity (Figure 2b), very similar curves are obtained for varying gas velocities, implying that the partial slip coefficient in quasi-2D beds is relatively insensitive to U/U_{mf}.

Figure 3 shows the variation of the coefficients *A* and *B* as a function of the coefficients of restitution and friction (Figure 3a) and the gas velocity (Figure 3b). It can be seen that the coefficient of friction has a stronger influence on the values of *A* and *B* than the coefficient of restitution. Both coefficients remain roughly constant over the range of gas velocities studied.

Comparison with the TFM

The new partial slip BC coefficient obtained from the DEM was implemented in the TFM. Figure 4 shows the solids volume fraction contour maps overlaid by the solids velocity vectors obtained from the DEM (Figure 4a), TFM simulation with the new BC (Figure 4b) and TFM simulation with the Johnson and Jackson BC (Figure 4c), of Case 1. The bed behaviour was found to be similar in the DEM and TFM with the new BC simulations. Concerning the solids motion, downflow close to the lateral walls and upflow in the middle of the bed can be observed in Figure 4a,b. Regarding the time-averaged values of the solids fraction, the DEM and TFM with the new BC simulations have similar patterns, i.e. a high solids concentration close to the lateral walls and uniform concentration in the middle of the bed, which is indicative of good solid mixing. In contrast, the TFM with the Johnson and Jackson BC shows a completely different flow behaviour.

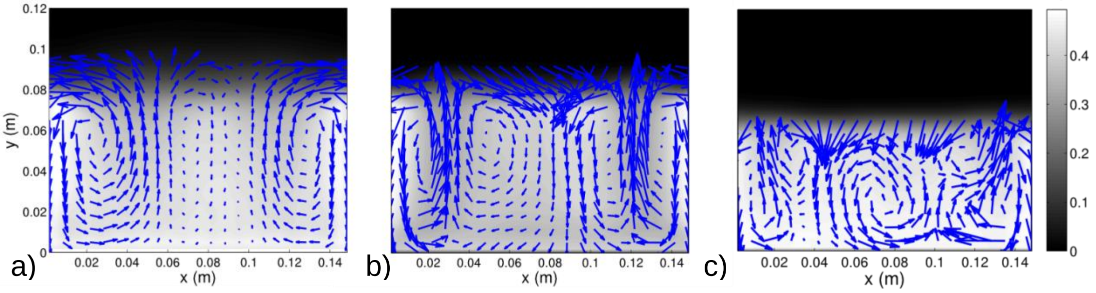

Figure 4: Solids volume fraction contour map overlaid with the solids velocity vectors: a) DEM simulation, b) TFM simulation with the new BC and c) TFM simulation with the Johnson and Jackson BC, Case 1.

The solids hold-up along the bed height and the vertical velocity of the solids at a height of 5.5 cm is shown in Figure 5 for the base case. Three different simulations are compared in the figure: the DEM simulation, the TFM with the new partial slip BC, Equation 3, and the TFM using the Johnson and Jackson BC (5). Figure 5a shows that the bed expansion obtained in the DEM and the TFM with the new BC simulations is similar, whereas the TFM with the Johnson and Jackson BC underestimates the trends of the DEM simulations. Regarding the solids velocity, Figure 5b confirms that the TFM simulations with the Johnson and Jackson BC predicts values of the same order of magnitude as the DEM simulations but the bed behaviour is different, showing 4 convection cells instead of the 2 cells observed in the DEM and the TFM with the new partial slip BC.

Further important features in fluidized beds are the bubble characteristics and dynamics. In order to study bubble motion, it is necessary to distinguish between bubbles and the emulsion phase. This was done by setting a cutoff value for the solids volume fraction equal to $\alpha_s = 0.3$ (Hernández-Jiménez et al. (3)), which is the arithmetic mean of the maximum and minimum solids volume fractions in the simulated bed. Any region in which the solids volume fraction was less than 0.3 was defined as a bubble. Figure 6 shows the mean bubble diameter versus the vertical position in the bed and the mean bubble velocity as a function of the bubble diameter. The standard deviations in these measurements are plotted as errorbars for the DEM and the TFM with the new BC simulations.

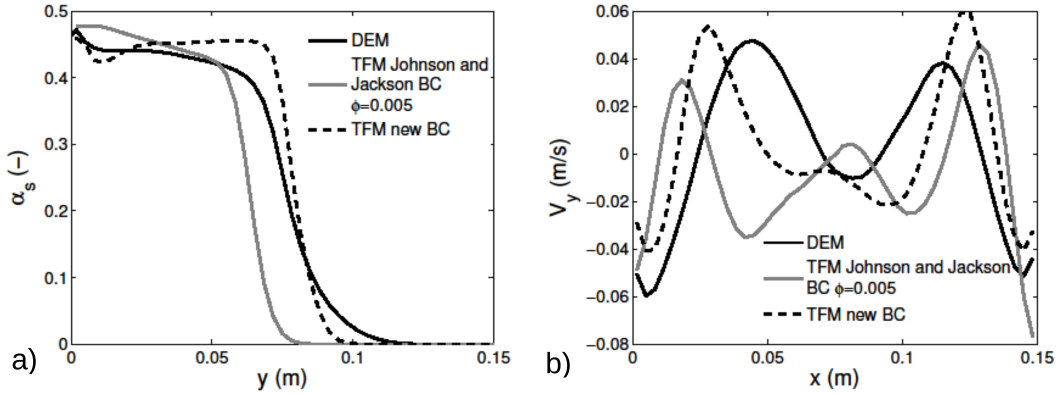

Figure 5: a) Solids hold-up along the bed height, and b) vertical solids velocity at a height of 5.5 cm above the distributor using the DEM, TFM with the new BC and TFM with the Johnson and Jackson BC. Case 1.

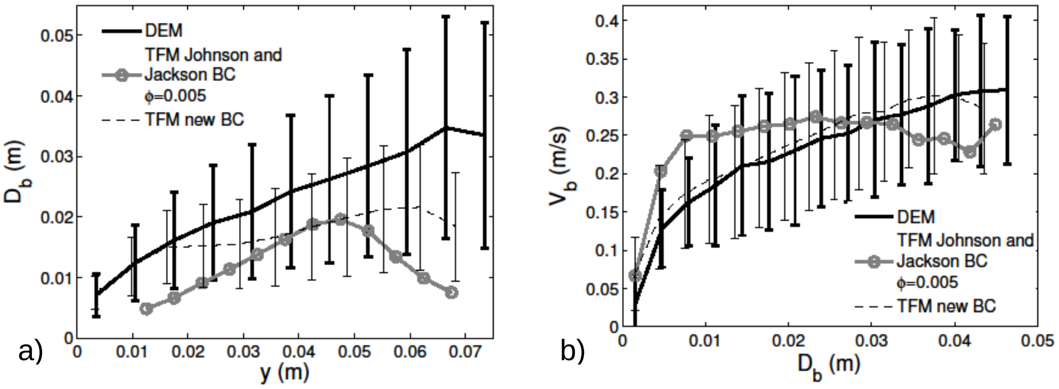

Figure 6: a) Bubble diameter versus vertical position, and b) bubble velocity in the vertical direction versus bubble diameter, for the DEM simulation and the TFM with the new BC and TFM with the Johnson and Jackson BC simulations, Case 1.

Figure 6a shows that the TFM with the new BC slightly underpredicts the bubble diameter compared to the DEM, but shows better results than those obtained with the TFM using Johnson and Jackson's BC. Regarding the bubble velocity (Figure 6b), both the DEM and the TFM with the new BC follow the same trend, whereas the bubble velocity predicted by the TFM with the Johnson and Jackson BC is almost independent of the bubble diameter.

CONCLUSIONS

A new boundary condition for the solid phase in pseudo-2D fluidized beds has been developed. This new BC was based on a partial slip equation fitted to DEM simulation data. Several particle parameters were tested to study their effect on the parameters of the new partial slip BC. The friction coefficient for particle-particle and particle-wall contacts was found to be the most important parameter. At low values of the solids volume fraction, the partial slip coefficient was found to be negative and, thus, contrary to the Johnson and Jackson BC (5). The new BC was implemented in a TFM and was shown to give more favourable results for quasi-2D beds than the classical Johnson and Jackson BC.

NOTATION

A , B	coefficients
D_b	bubble equivalent diameter (m)
e	coefficient of restitution (-)
U	superficial gas velocity (m/s)
U_{mf}	min. fluidization velocity (m/s)
V_b	bubble velocity (m/s)
$\overrightarrow{V_s} = (V_x, V_y)$	solids velocity (m/s)
V_{wall}	solids velocity at the wall (m/s)
α_s	solids volume fraction (–)
ρ_s	solids density (kg/m^3)
ϕ	coefficient of friction

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