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Improvement of the simulation of fuel particles motion in a fluidized bed by considering wall friction

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Abstract

The mixing of fuel particles is a key issue on the performance of fluidized bed reactors. In this work, the motion of a non-reactive fuel particle in a pseudo-2D bubbling fluidized bed operated at ambient conditions is simulated employing a hybrid-model and introducing a new friction term that accounts for the effect of the bed vessel front and rear walls. The hybrid-model, implemented in the code MFIX, simulates the dense and gas phases using a Two-Fluid Model (TFM) whereas the fuel particles are modeled using a Discrete Element Method (DEM). The importance of the present hybrid-model is that the interaction of the continuum phases with the fuel particles behavior is fully coupled.

To improve the accuracy of the simulated fuel particle motion in a bubbling fluidized bed, a model accounting for the effect of the bed front and rear walls on the continuum solid phase is combined with the hybrid-model. The rising and sinking velocity of the fuel particles, the circulation time and statistical parameters associated to the location of the fuel particle in the bed were obtained from the simulations and compared with experimental measurements. According to the results, the prediction of these parameters is clearly improved when the friction term is included in the simulation.

Keywords: Fuel motion, mixing, bubbling fluidized bed, hybrid-model, wall friction.

1. Introduction

Fluidized beds are characterized by a high thermochemical conversion of solid fuel particles due to their great heat and mass transfer efficiency [1]. The study of the mixing of fuel particles in the whole bed during thermal conversion processes is a key issue for the proper design of a fluidized bed reactor [2]. The fuel particle mixing is characterized by the time spent by the fuel particle in the bed (i.e. the residence time), the capability of the fuel particle to move in the horizontal and vertical directions, (i.e. the axial and lateral dispersion) and the time needed for its thermochemical conversion (i.e. the thermochemical conversion time).

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Several experimental works present in the literature are focused on the motion of fuel particles in pseudo-2D and 3D fluidized beds. Pseudo-2D fluidized bed systems typically have a transparent front wall to allow optical access to the system and the rear wall of the bed is separated to the front wall by a narrow distance to ensure that the visualization is representative of the whole system. In most of the studies available in the literature, the tracer particles are considered as objects, varying in density, shape and/or size to the bed material. It was observed that these objects sink to the bottom of the bed close to its lateral walls, following the motion of the dense phase, and rise through the center of the bed, affected by the bubbles ascension [3, 4, 5, 6, 7]. This motion pattern is characteristic of bubbling fluidized beds composed of a single mixing cell [5]. Additionally, the rising process of an object consists in a series of small jumps due to the effect of different passing bubbles [8]. This phenomenon was also experimentally characterized by Soria-Verdugo et al. [6] using a neutrally buoyant object, i.e. an object with a density similar to that of the bed bulk, and objects with different densities and sizes [9], provided that the objects showed a proper circulation throughout the whole bed. Furthermore, Soria-Verdugo et al. [9, 10] studied, in pseudo-2D and 3D lab-scale fluidized beds, the influence of the density and size of the objects on their circulation time in the bed. In a very similar system, Garcia-Gutierrez et al. [11] showed that fuel particles follow a ballistic path when they are ejected by the bubbles in the freeboard, which means that fuel particles motion out of the dense bed is only affected by gravity. Other related works have used a Monte Carlo method to reproduce the motion of fuel particles inside a pseudo-2D bed [12] and the behaviour of a fuel particle in a industrial reactor, obtaining results in very good agreement with experimental results available in the literature [13].

Complementary to the experimental studies, numerical simulations, either Eulerian-Eulerian Two-Fluid Models (TFM) [14, 15, 16], Eulerian-Lagrangian approaches such as discrete element models (DEM) [17, 18], or a combination of both strategies (coupled TFM-DEM) [19], can be a very effective complementary tool to experiments to achieve a detailed analysis of the hydrodynamics of complex gas-solids systems such as fluidized beds [20, 21]. In the TFM approach, the gas phase and the particles or solids phase are treated as two interpenetrating continua in an Eulerian framework, using the conservation equations of fluids. The DEM strategy is based on a Lagrangian simulation of each particle trajectory coupled with an Eulerian simulation of the bulk gas flow. In the coupled TFM-DEM hybrid model, the gas and solid phases are modeled as two interpenetrating continua combined with the simulation of discrete particles. This strategy has demonstrated to be of great interest for the simulation of particle segregation [22, 23]. Due to its unique characteristics, the coupled TFM-DEM hybrid model can be also employed to characterize the motion of fuel particles inside the bed. In a previous work, Hernández-Jiménez et al. [19] used this hybrid model to compare simulation results of the motion of a fuel particle with experimental data extracted from the literature [6]. The comparison showed great accordance in the results related to the location of the fuel particle in its motion throughout the whole bed.

Furthermore, Li et al. [24] and Hernández-Jiménez et al. [25] reported that the effect of the front and the

rear walls on the particles motion can be significant and should not be neglected in numerical simulations of pseudo-2D beds. The wall effect in numerical simulations of gas-solids pseudo-2D systems has been investigated in several numerical studies using either TFM or CFD-DEM models, demonstrating its relevance [26, 27, 28, 29, 30]. Recently, Hernández-Jiménez et al. [31] developed an empirical model to easily account for the particle-wall interaction effect in pseudo-2D fluidized beds. The model allows for the simulations of the wall-friction effect in pseudo-2D beds using a 2D domain instead of a more computationally demanding 3D domain. The results obtained by Hernández-Jiménez et al. [31] showed that the incorporation of the wall-friction model produces a clear improvement of conventional 2D simulations.

In the present work, the motion of a fuel particle in a pseudo-2D bubbling fluidized bed is simulated employing a hybrid TFM-DEM model and introducing the new friction term associated to the wall effect proposed by Hernández-Jiménez et al. [31]. Therefore, in this work, the effect of the change of the fluid-dynamics of the bed, produced by friction of the dense phase with the front and rear walls, on the motion of fuel particles is considered for the first time. This novel numerical approach permits to increase the predictive capabilities of the fully coupled TFM-DEM model previously described in [19]. The simulation results were compared with the experimental evidences obtained by Soria-Verdugo et al. [6, 9] and with simulations without considering the wall friction term of the front and rear walls, similarly to the results analyzed in [19]. Statistical parameters concerning the location, the sinking and rising velocity and the circulation time of the fuel particle are analyzed. To study the influence of the fuel particles density, two different densities of fuel particles were studied in the simulations. The comparison between the simulations and the experimental results for both fuel particles shows a significant improvement of the predictive capabilities of the simulations when the new friction term is accounted for. This improvement is of central importance, since a proper description of the time dependant parameters by the simulations is critical to model the thermochemical reaction of the fuel particles in fluidized bed reactors.

2. Simulation

2.1. Theory

The open-source MFIX-Hybrid code, developed at US Department of Energy's National Energy Technology Laboratory, was used to conduct the numerical simulations of a 2D bubbling fluidized bed. In the MFIX-Hybrid code, an Eulerian-Lagrangian-Eulerian approach is employed. The gas phase is treated as continuum, and the different solid phases can be treated either as continuous (Eulerian) or discrete (Lagrangian). In the present work, the gas and dense (bed material) phases are treated as continuum and the fuel particles introduced in the bed are modeled as discrete inert entities.

The continuum description of the gas and dense phases, i.e. Two-Fluid Model, is based on the equations of mass and momentum conservation and granular temperature balance [32, 33]. In the discrete description

of the present study, the fuel particles are represented as individual particles in the flow, and inter-particle collisions are directly solved using the soft-sphere approach proposed by Cundall and Strack [34] and Tsuji et al. [35].

The governing equations of the hybrid model are summarized in the following lines. The subscript s is referred to the solid continuum phase, g to the gas phase and p to the discrete fuel particles.

Mass conservation of the gas and solid phases, continuum:

$$\frac{\partial}{\partial t}(\alpha_g \rho_g) + \nabla \cdot (\alpha_g \rho_g \vec{v}_g) = 0 \quad (1)$$

$$\frac{\partial}{\partial t}(\alpha_s \rho_s) + \nabla \cdot (\alpha_s \rho_s \vec{v}_s) = 0 \quad (2)$$

Momentum conservation of the gas phase, continuum:

$$\begin{aligned} \frac{\partial}{\partial t}(\alpha_g \rho_g \vec{v}_g) + \nabla \cdot (\alpha_g \rho_g \vec{v}_g \vec{v}_g) = \\ -\alpha_g \nabla p_g + \nabla \cdot \overline{\overline{\tau}}_g + \alpha_g \rho_g \vec{g} + K_{gs}(\vec{v}_s - \vec{v}_g) + K_{pg}(\vec{v}_p - \vec{v}_g) \end{aligned} \quad (3)$$

Momentum conservation of the solid phase, continuum:

$$\begin{aligned} \frac{\partial}{\partial t}(\alpha_s \rho_s \vec{v}_s) + \nabla \cdot (\alpha_s \rho_s \vec{v}_s \vec{v}_s) = \\ -\alpha_s \nabla p_g - \nabla p_s + \nabla \cdot \overline{\overline{\tau}}_s + \alpha_s \rho_s \vec{g} - \vec{f}_{fric} + K_{gs}(\vec{v}_g - \vec{v}_s) + K_{ps}(\vec{v}_p - \vec{v}_s) \end{aligned} \quad (4)$$

where p_i is the pressure and $\overline{\overline{\tau}}_i = \alpha_i \mu_i (\nabla \vec{v}_i + \nabla \vec{v}_i^T) + \alpha_i (\lambda_i - \frac{2}{3} \mu_i) \nabla \cdot \vec{v}_i \vec{I}$ is the stress tensor for phase i .

To account for the effect of the front and rear walls of the pseudo-2D bed, the extra body force term \vec{f}_{fric} is incorporated in Equation 4, as proposed by Hernández-Jiménez et al. [31]. This term can be neglected for the gas phase as it is expected to have a comparatively minor effect. This extra body force, per unit of volume of the bed, is expressed as:

$$\vec{f}_{fric} = \frac{2c\vec{v}_s}{Z} \quad (5)$$

where c is an empirical coefficient [31], Z is the bed thickness and \vec{v}_s is the solids velocity vector, which is assumed to be equal in both the front and rear walls and equal to the central plane vector velocity in a pseudo-2D bed. Equation 6 is used to calculate the coefficient c in Equation 5, as developed by Hernández-Jiménez et al. [31]. Further details about the development and implementation of the term \vec{f}_{fric} can be found in [31].

$$c = 6.2 \frac{d_s^2 \rho_s g^{1/2}}{Z^{3/2}} + 5.6 \cdot 10^{-2} \rho_s Z^{1/2} g^{1/2} \quad (6)$$

Finally, the balance for the granular temperature, Θ , is:

$$\begin{aligned} \frac{3}{2} \left(\frac{\partial}{\partial t} (\rho_s \alpha_s \Theta) + \nabla \cdot (\rho_s \alpha_s \vec{v}_s \Theta) \right) = \\ (-p_s \bar{\bar{I}} + \bar{\bar{\tau}}_s) : \nabla \vec{v}_s + \nabla \cdot (k_\Theta \nabla \Theta) - \gamma_\Theta - 3K_{gs} \Theta \end{aligned} \quad (7)$$

where $(-p_s \bar{\bar{I}} + \bar{\bar{\tau}}_s) : \nabla \vec{v}_s$ is the generation of Θ by the solids stresses, $k_\Theta \nabla \Theta$ is the diffusion of Θ , γ_Θ is the collisional dissipation of Θ and $3K_{gs} \Theta$ is the transfer of random kinetic energy between the solids and the gas. In Equations 3, 4 and 7, K_{gs} is the drag force between the gas and the solid phase. For simplicity, the effect of the front and rear walls on the net production of granular temperature in the bed is not considered here, as it has been proven to have a negligible effect on the velocity profiles [29]. The drag force correlation for the gas–solid interaction used in this work is the one proposed by Gidaspow [15].

The position, \vec{X} , the linear velocity, \vec{V} , and the angular velocity, $\vec{\omega}$, of the different discrete particles, j , evolve according to Newton's laws of motion as:

$$\frac{d\vec{X}^j}{dt} = \vec{V}^j \quad (8)$$

$$m^j \frac{d\vec{V}^j}{dt} = \vec{F}_T^j = m^j \vec{g} + \vec{F}_d^j + \vec{F}_c^j \quad (9)$$

$$I^j \frac{d\vec{\omega}^j}{dt} = \vec{T}^j \quad (10)$$

where m^j and I^j are the mass and moment of inertia of each j particle, \vec{F}_c^j is the net contact force on a particle as a result of its contact with other discrete particles. \vec{F}_c^j also includes the net force produced by the collisions of the continuous solids phase with the discrete particles given by $K_{ps}(\vec{v}_s - \vec{v}_p)$. \vec{F}_d^j is the total gas–solid drag force (pressure and viscous) on each particle j produced by the solids phase (bed material), and \vec{F}_T^j is the net sum of all forces acting on each j particle. \vec{T}^j is the net torque due to the tangential component of the contact forces acting on each j particle, exerted by other solid particles (continuum or dense) or walls.

The drag force proposed by Gidaspow [15] correlation for all the gas–solid interactions, K_{gs} and K_{pg} , is selected in this work. For the particle–solids phase interaction, the coefficient K_{ps} derived by Syamlal [36] as a simplified version of the kinetic theory is used in the present simulations:

$$K_{ps} = \frac{3(1 + e_{sp})(\pi/2 + C_{sp}\pi^2/2)\alpha_p\rho_p\alpha_s\rho_s(d_s + d_p)^2 g_{0,sp}|\vec{v}_s - \vec{v}_p|}{2\pi(\rho_p d_p^3 + \rho_s d_s^3)} \quad (11)$$

where e_{sp} and C_{sp} are, respectively, the coefficients of restitution and friction between the solids phase and the discrete particles. The radial distribution function at contact, $g_{0,sp}$, was that derived by Lebowitz [37] for a mixture of hard spheres of different sizes:

$$g_{0,sp} = \frac{1}{\alpha_g} + \frac{3d_p d_s}{\alpha_g^2(d_p + d_s)} \sum_{\lambda=1}^M \frac{\alpha_{s\lambda}}{d_{p\lambda}} \quad (12)$$

where λ goes from 1 to M , being M the total number of solids phases, discrete and continuum.

The friction term incorporated in Equation 4 is not included in the discrete description since these forces can be considered negligible for the fuel particles. Garcia-Gutierrez et al. [11] experimentally demonstrated in a pseudo-2D fluidized bed that fuel particles follow a ballistic path when they are ejected by bubbles in the freeboard, which means that the motion of fuel particles out of the dense bed is mainly affected by gravity and thus the friction with the front and rear walls is negligible. This implies that inside the dense bed, the motion of the fuel particles will be primarily affected by the interaction with the gas and continuous solid phases.

2.2. Simulated system

The system simulated is a pseudo-2D cold bubbling fluidized bed with the same characteristics as that employed by Soria-Verdugo et al. [6] in their experiments. The experimental facility consists of a fluidized bed of 0.5 m width, W , 1.5 m of height, H , and 0.01 m of thickness, Z . Due to the two-dimensionality of the bed, the fuel particle motion occurs only in the horizontal and vertical directions, thus the simulation only covers two dimensions, i.e. 2D domain (0.5 m x 1.5 m). The simulated bed material was spherical particles with a particle density of $\rho_s = 2500 \text{ kg/m}^3$ and an average particle diameter of $d_s = 700 \mu\text{m}$, which is similar to that employed by Soria-Verdugo et al. [6]. It is important to remark that the bed material and the gas phase are simulated as continuum phases while the fuel particle is modelled as a discrete entity. For simplicity, the fuel particle is assumed to be a circular particle with the same mass as the cylindrical shaped particle tested by Soria-Verdugo et al. [6]. Two fuel particles with different densities are simulated to study the buoyancy effects in the simulation. The densities chosen represent fuel particles with neutrally buoyant ($\rho_p = 1508 \text{ kg/m}^3$) and flotsam ($\rho_p = 1230 \text{ kg/m}^3$) behaviours, both referred to the bulk density of the bed ($\rho_b = 1560 \text{ kg/m}^3$). These fuel particles present a proper circulation movement throughout the whole bed according to Soria-Verdugo et al. [9]. To increase the amount of data obtained in each of the numerical cases, for later statistical analysis, three identical discrete particles were simulated simultaneously

Table 1: Simulation parameters.

Bed material and gas characteristics	
Bed height, H [m]	1.5
Bed thickness, Z [m]	0.01
Bed width, W [m]	0.5
Static bed height, h_0 [m]	0.5
Bed material density, ρ_s [kg/m ³]	2500
Bed material diameter, d_s [μ m]	700
Minimum fluidization velocity, U_{mf} [m/s]	0.32
Dimensionless gas velocity, U/U_{mf} [–]	2.5
Gas density, ρ_g [kg/m ³]	1.2
Coefficient of restitution, $e_s = e_{sp}$ [–]	0.9
Angle of internal friction, Φ [deg]	30

for each case. The particles started the simulation at different horizontal but in the same vertical positions in the freeboard of the bed and they are individually tracked. The number of collisions between the three discrete particles analyzed simultaneously is below 0.02 per second, assuring an independent motion of the fuel particles in the bed.

The parameters employed in the simulations of the continuum phase (bed material and fluidizing gas) and the fuel particles characteristics are summarized in Table 1 and Table 2, respectively.

The new simulations with the wall friction term were developed for two different fuel particle densities and the results were compared with simulations without the friction term and with experimental data obtained from Soria-Verdugo et al. [6, 9]. The superficial gas velocity employed in the simulations is $2.5U_{mf}$ for all the cases, as for the experimental tests. The nomenclature employed for the different cases studied is shown in Table 3. In this table, the abbreviations N and F refer to the neutrally buoyant behaviour and to the flotsam behaviour of the fuel particle, respectively.

The 2D computational domain is discretized using a uniform grid with cells of $\Delta s = 5$ mm size in the horizontal and vertical directions (100 x 300 cells). This grid size is considered small enough to ensure grid independent results [24, 31]. The gas flow is fed uniformly through the bottom of the bed using a velocity inlet boundary condition, which represents an air supply system fully uncoupled from the bed. In the experiments by Soria-Verdugo et al. [6] a gas distributor with a characteristic constant equal to $8200 \text{ Pa}/(\text{m/s})^2$ is used. This ensures, for the cases studied here, a large distributor-to-bed pressure ratio and, therefore, a homogeneous distribution of the air throughout the whole bed [38]. The gas flow leaves the system through the top boundary at a constant pressure. A no-slip boundary condition is used for the gas and continuum solid phases at the side walls of the bed. Besides, previous works have demonstrated that the lateral boundary condition does not have a strong effect in this kind of simulations [24, 39].

Table 2: Fuel particle characteristics.

Discrete fuel particles parameters	
Density, ρ_p [kg/m ³]	
Flotsam particle, F	1230
Neutrally buoyant particle, N	1508
Particle diameter, d_p [cm]	1.06
Normal inter-particle spring constant [N/m]	1000
Tangential inter-particle spring constant [N/m]	286
Normal wall-particle spring constant [N/m]	1000
Tangential wall-particle spring constant [N/m]	286
Particle-particle friction coefficient [-]	0
Particle-wall friction coefficient [-]	0
Particle-particle restitution coefficient [-]	0
Particle-wall restitution coefficient [-]	0
Coefficient of friction between unlike solids, C_{sp} [-]	0.1

Table 3: Cases studied.

	Discrete particle density [kg/m ³]	
	1230 (F)	1508 (N)
Simulation without friction term	SIM	SIM
Experimental data	EXP	EXP
Simulation with friction term	SIM fric	SIM fric

3. Results

The results presented in this work are divided in three main sections. In the first section, the effect of including the friction term in the simulation on the bubble distribution in the bed is studied. In the second section, the results presented are devoted to the location and behaviour of the fuel particles in the fluidized bed. Finally, the third section focuses on the motion of the fuel particle related to the time scale, i.e. the time spent by the fuel particle inside the dense bed and the velocities in its sinking and rising processes. In all the sections, the results compare the experimental results with standard simulations and with simulations considering wall friction.

3.1. Bubbles distribution in the bed

The preferential path of bubbles during their ascension to the bed surface directly affects the motion of the particles inside the fluidized bed. The presence of larger bubbles in the system implies a higher coalescence rate. This phenomenon modifies the dynamics and the time of the rising and sinking processes of fuel particles in the dense bed. To evaluate the effect of the friction term on the bubbles distribution and, subsequently, on the motion of the fuel particle inside the bed, the solids fraction at each point of the bed was calculated. Figure 1 shows the normalized time-averaged maps of the solids volume fraction, $\bar{\alpha}_s$, extracted from simulations without (Figure 1a) and with (Figure 1c) the friction term and that obtained in the experiments [6] (Figure 1b). In the figure, $\bar{\alpha}_s = 1$ corresponds to the maximum solids volume fraction and $\bar{\alpha}_s = 0$ to the minimum solids volume fraction, so that the simulation and experimental results can be directly compared. Note also that the numerical results are continuous whereas the experimental data can only take discrete values (0 or 1), once the images of the bed are binarized. This means that points with an intermediate value of solids concentration will be slightly overestimated in the experimental results. The time-averaged solids volume fraction was obtained by averaging, during 150 s (starting 10 s after the start-up), the instantaneous volume fraction of the simulations.

A preferential bubble path can be observed in Figure 1 both for the experimental and the numerical cases, regardless of the consideration of the friction term. Therefore, both simulations, neglecting and considering the friction term, are capable of describing the global behaviour of bubbles in the bed. The results obtained for the case of the simulation including the friction term (Figure 1c) are very similar to the experimental results (Figure 1b), obtaining in both cases the bubble eruption region in a zone close to $y \sim 60$ cm. However, for the case of the simulation without the friction term (Figure 1a) the bubble eruption region is located at a lower height, around $y \sim 55$ cm. In fact, the average bed height, \bar{h}_{fb} , obtained from the simulation neglecting the friction term is 58.5 cm, whereas for the simulations considering the friction term is 61.5 cm coinciding with the value obtained from the experiments ($\bar{h}_{fb} = 61,5$ cm). This averaged bed height is obtained by thresholding the time averaged solids volume fraction maps to discriminate the time

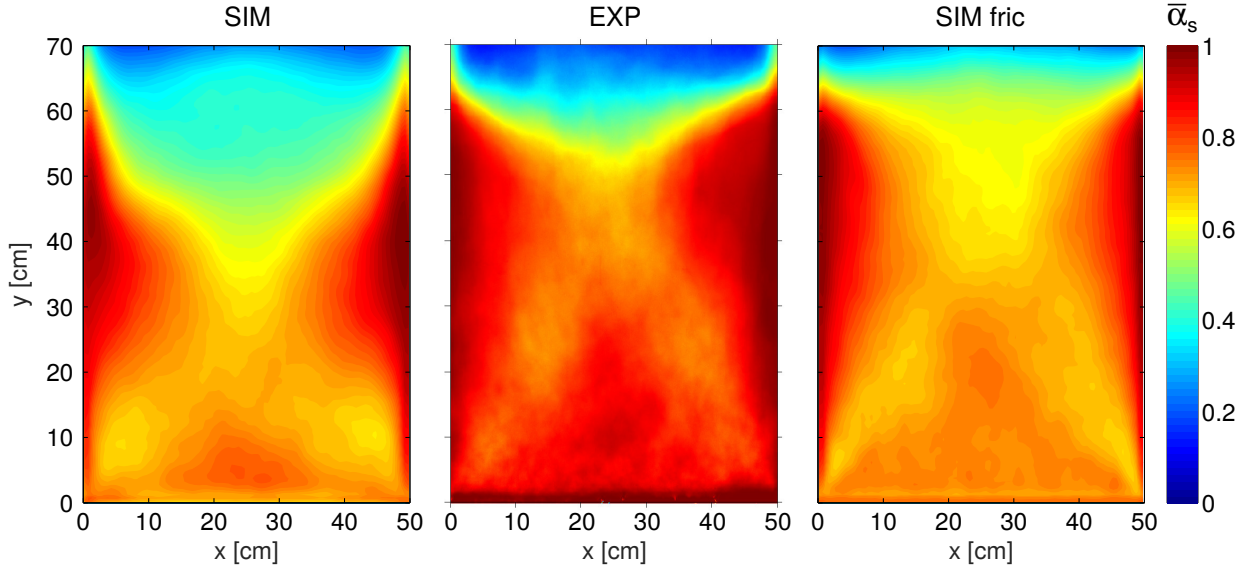


Figure 1: Normalized time-averaged solids volume fraction for a) the simulation without the friction term, b) experiments of Soria-Verdugo et al. [6] and c) the simulation with the friction term.

averaged bed surface and performing then a spatial average over the horizontal direction. This discrepancy in the averaged bed height indicates that neglecting the friction term in the simulation leads to a different overall bed behaviour, promoting bubbles coalescence and presenting a clearly marked preferential bubble path along the whole bed.

To analyze the differences on the bubble coalescence between the experimental and the two different simulation results, the average bubble size distribution as a function of the bed width was studied. Figure 2 shows the mean bubble diameter along the bed width for both the experimental and the simulated systems. Even though the experimental data is not reported in Soria-Verdugo et al. [6], it has been calculated from the experimental measurements analyzed to be compared with the simulation results here presented. In Figure 2, the mean bubble diameters are similar on the sides of the bed for the experiments and the simulations. However, in the middle of the bed, where the preferential path of the bubbles is located, the mean bubble diameter increases considerably for the simulation without the friction term. The simulation with the friction term shows mean bubble diameters similar to those of the experimental results along the whole bed width. This result, in combination with those presented in Figure 1, reveals the presence of larger bubbles in the preferential path located at the center of the bed for the simulation without the friction term compared to the simulation with the friction term. This also implies different fuel particle behaviors between both simulations. Moreover, the experimental results and the results of the simulation with the friction term show a great similitude in terms of the bubble behaviour, improving considerably the results obtained in the simulation without the friction term. This fact was already concluded by Hernández-Jiménez et al. [31] for different fluidized beds and operational conditions.

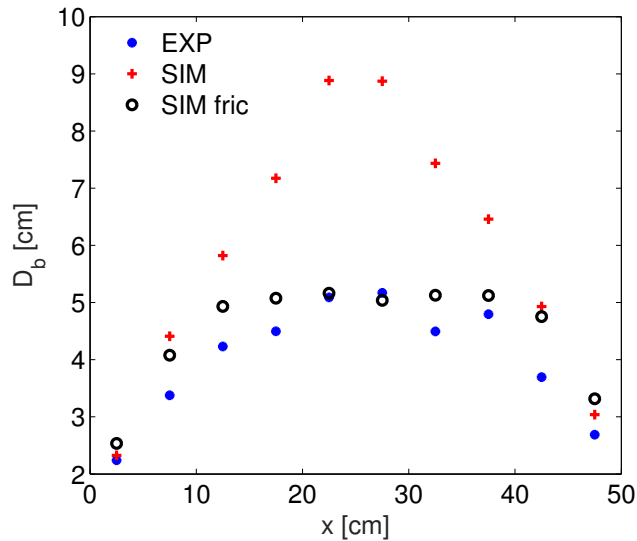


Figure 2: Mean bubble diameter, D_b , along the bed width, x , for the experimental results obtained by Soria-Verdugo et al. [6], simulation results without the friction term and simulation results with the friction term.

3.2. Location of the fuel particle in the bed

The location of the fuel particle in the bed was numerically studied in a preliminary work by Hernández-Jiménez et al. [19] by means of the TFM–DEM hybrid model in which the effect of the front and rear walls was not accounted for. The simulation showed good agreement with the experimental results reported by Soria-Verdugo et al. [6]. In the present work, the relative frequency of finding the fuel particle at a certain height was calculated in the simulation including the new wall friction term and for two different fuel particle densities. The results were compared with the original simulation without the friction term and with the experimental results obtained by Soria-Verdugo et al. [6, 9]. These results are presented in Figure 3a for a fuel particle with flotsam behaviour ($\rho_p = 1230 \text{ kg/m}^3$) and in Figure 3b for a neutrally buoyant behaviour fuel particle ($\rho_p = 1508 \text{ kg/m}^3$). Note that the results shown in Figure 3a are not reported in [9] but they were obtained from the experimental data presented there.

Regarding the flotsam fuel particle, the results obtained in the simulation with the new wall friction term provide a better prediction of the vertical location of the fuel particle than the simulation without the friction term, as can be seen in Figure 3a. The largest discrepancy between the standard simulation without the friction term and both the experiments and the simulation accounting for the wall friction is observed in the splashing zone, where the bubbles erupt, i.e. close to the fixed bed height. In this zone (between $y = 45 \text{ cm}$ and $y = 80 \text{ cm}$) the Mean Square Error (MSE) between the simulations and the experimental results is 0.26 for the simulation without considering the wall friction and it is reduced to 0.07 for the simulation with the friction term. Besides, when the fuel particle is located at the lower region of the bed, the values of the MSE are 0.12 and 0.09 for the simulation neglecting and considering the friction term, respectively. The

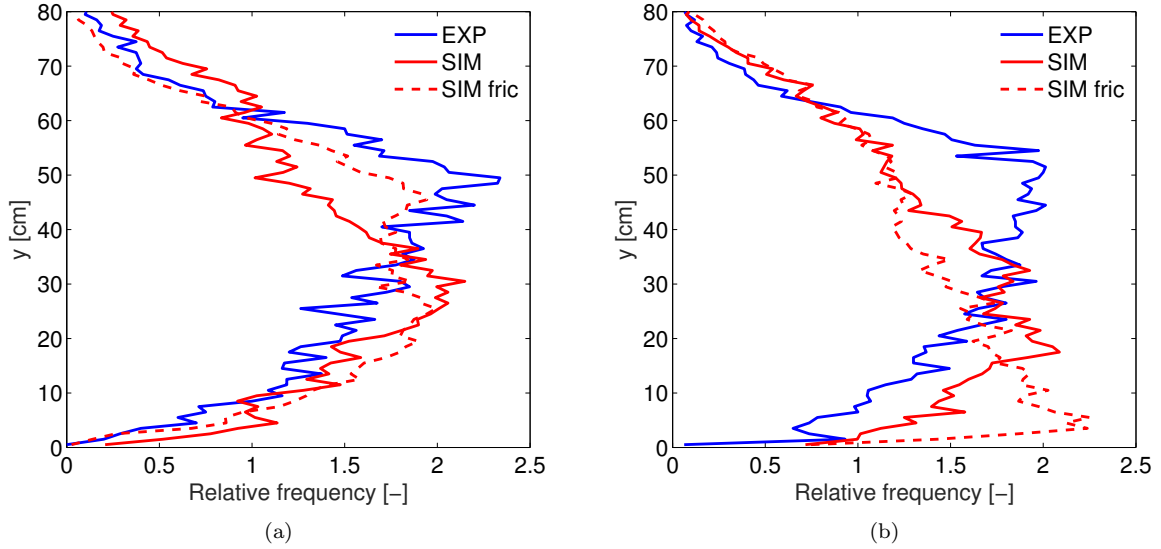


Figure 3: Relative frequency of finding the fuel particle at a certain height. a) Flotsam behavior. b) Neutrally buoyant behavior.

differences encountered in the splashing zone can be attributed to the higher bubble coalescence obtained when neglecting the friction term in the simulation, obtaining a more pronounced bubble preferential path with a lower height of the splashing zone (Figure 1a), and larger bubbles at the center of the bed (Figure 2). This also causes the fuel particle to reach the freeboard quickly, as it is easily dragged upwards by the presence of larger bubbles.

In the case of the neutrally buoyant behavior, both kind of simulations overestimate the relative frequency of the fuel particle at the bottom of the fluidized bed. This discrepancy can be attributed to the similar density between the fuel particle and the bed bulk. This implies that when the fuel particle reaches the bottom of the bed, bubbles might not be large enough to drag it upwards again, so the circulation of the fuel particle is deteriorated. In the experiments, this issue is less common because of the distributor employed. The perforated plate used in the experiments creates small jets at the bottom of the bed, rather than very small bubbles. The gas velocity of these jets might be high enough to effectively lift the fuel particle to a height at which bubbles are able to rise it.

Another parameter commonly used to characterize the motion of fuel particles in a fluidized bed is the number of bubbles needed by the fuel particle to reach the bed surface in a cycle, moving from the bed surface to a determine depth and back to the surface. This number of bubbles needed to raise the fuel particle to the bed surface is the so-called number of jumps. Soria-Verdugo et al. [6, 9] determined experimentally the relative frequency of the number of jumps needed by a fuel particle to reach the bed surface, P_{N_j} , and described this behaviour with a geometrical equation, as shown in Equation (13):

$$P_{N_j} = p(1 - p)^{N_j - 1} \quad (13)$$

where N_j is the number of jumps and $p = 0.45$ is a fitting parameter corresponding to the probability of a bubble, to which the fuel particle is attached, to raise directly to the bed surface. This value of $p = 0.45$ was experimentally obtained for several objects with different sizes and densities [6, 9].

Figure 4 presents the values of P_{N_j} obtained experimentally and from the different simulations and fuel particle densities. Also, Figure 4 includes the geometrical fitting of Equation (13), with $p = 0.45$, obtained experimentally by Soria-Verdugo et al. [6].

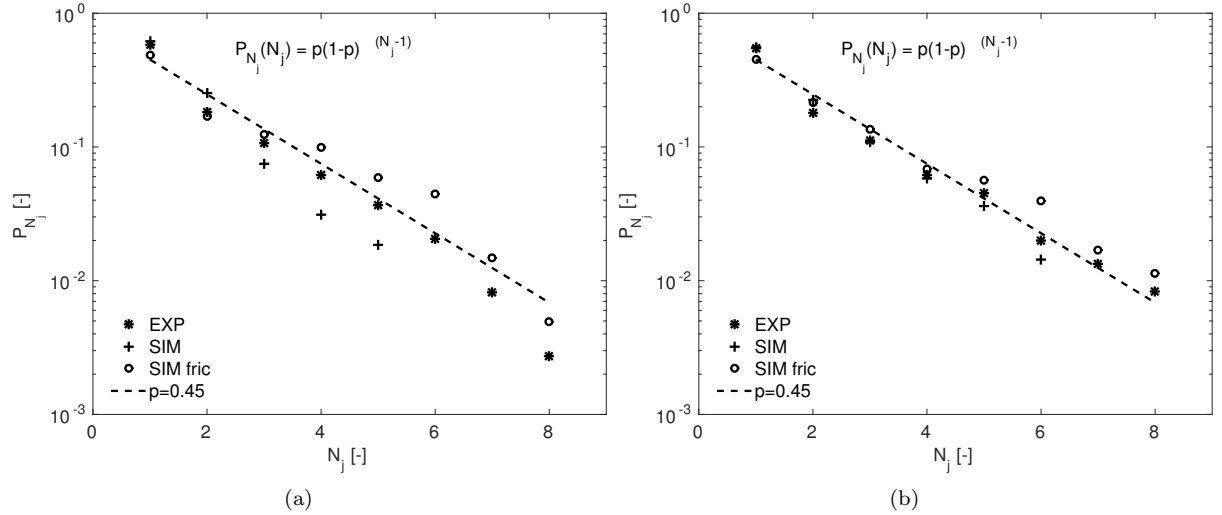


Figure 4: Probability of the number of jumps needed by the fuel particle to reach the bed surface in a cycle. a) Flotsam behavior. b) Neutrally buoyant behavior.

The results obtained from the fuel particle density of 1232 kg/m^3 are presented in Figure 4a. A fairly good agreement between the experimental and the simulation results in the fitting of the equation can be observed in the figure. Besides, in the simulations without the friction term, the maximum number of jumps employed by the fuel particle to reach the bed surface in a cycle were 5, which is smaller than the maximum number of jumps needed in the simulation with the friction term and in the experiments. The same behaviour was observed for the neutrally buoyant fuel particle (Figure 4b), where the maximum number of jumps obtained by the simulation without the friction term was 6. As in the case of Figure 3, these discrepancies between the simulations without friction for both fuel particles can be associated to the results discussed in Figures 1 and 2. These correspond to the more pronounced preferential path of bubbles and the larger bubble size in this path for the simulations without the friction term (Figure 1 and Figure 2). This causes that fuel particles are more easily dragged by the larger bubbles rising in the bed, which

reduces the number of bubbles, i.e. the number of jumps, needed for the particle to rise back to the bed surface. Both the geometrical fitting and the maximum number of jumps needed are better reproduced by the simulations including the friction term.

3.3. Time scale results

From a practical point of view, it is of great interest to study the fuel particle velocity and the circulation time spent by the particle in its motion inside the dense bed. Note that the motion of an object immersed in the dense bed is associated, during the ascending process, to the rising of bubbles in the bed, and, during the sinking process, to the motion of the dense phase. Fuel particles in a range of densities similar to the density of the bed bulk tend to move accordingly to the motion of the dense phase throughout the whole bed, since buoyancy forces are not relevant. On the other hand, objects with densities much larger than the density of the bed bulk tend to sink to the bottom of the bed and remain stagnant in that region. Symmetrically, objects with much lower densities than the density of the bed bulk tend to float over the bed surface or stay in the upper section of the bed [1, 6, 9, 10].

The capability of the simulations to reproduce the fuel particle velocity during the rising and sinking processes was evaluated by comparing the simulation results with the experimental data and with the theoretical mean bubble velocity and dense phase downwards velocity. These theoretical values were calculated using the well-known correlations of Davidson and Harrison [40] and Kunii and Levenspiel [1], for the bubbles and the dense phase velocity, respectively, using the same operating values of the bed as in the experiments (see Table 1). Further details on the calculation of the bubbles and dense phase velocities can be found in [6, 7, 9]. Figure 5 shows the results of the fuel particle velocity for the experiments and the simulations with and without the wall-friction term. In Figure 5a, the fuel rising velocity was related to the 20% [6, 7] of the bubble velocity and the fuel sinking velocity was compared to the dense phase downwards velocity [6, 9]. The sinking velocity depicted in Figure 5b was obtained by removing from the data analysis the downwards velocity associated to the vibration of the fuel particles in their sinking path, according to Soria-Verdugo et al. [6]. This implies the application of a sampling frequency of 2 Hz in the simulations, the same sampling frequency employed in the experimental data.

It can be observed in Figure 5a that the wall friction term considerably improves the results of the fuel particle rising velocity with regard to the simulations neglecting the wall friction term. The fuel particle rising velocity for the case considering wall-friction is very similar to 20% the bubble velocity and to the experimental data. Regarding the sinking velocity of the fuel particle shown in Figure 5b, the simulation with the friction term also improves the results obtained from the standard simulation. However, there is a slight difference with the dense phase downwards velocity obtained from the correlation and the experimental results. Despite of these slight discrepancies, the wall friction term included in the simulations is capable of determining more accurately the mean fuel particle velocity both during the sinking and the rising

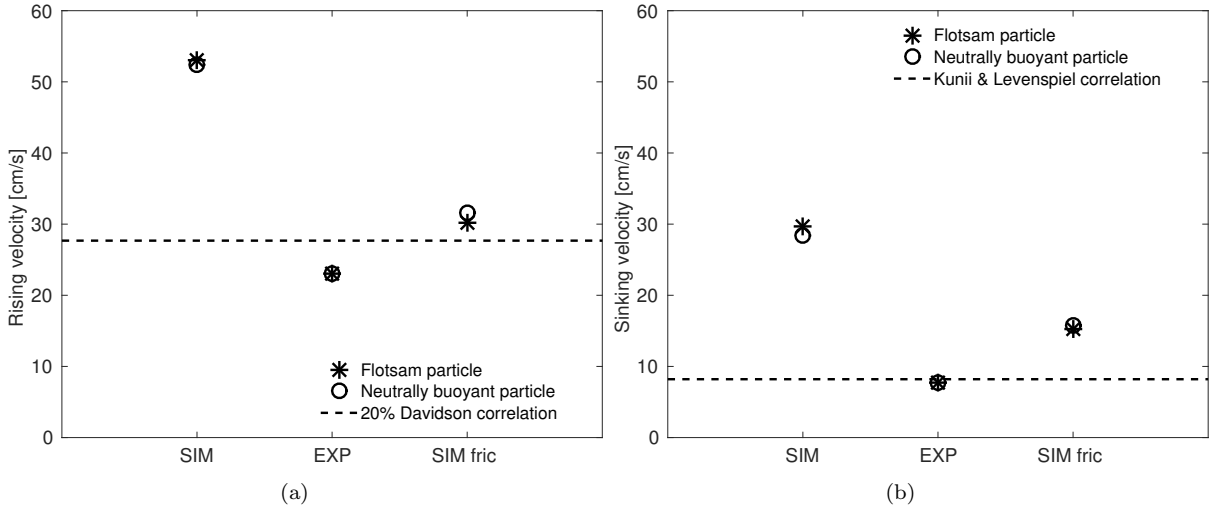


Figure 5: Comparison of the mean fuel particle velocity during a) the rising process and b) the sinking process.

processes. The discrepancies observed in the rising and sinking velocities when neglecting the friction term in the simulation may be attributed to the differences observed in the bubble preferential path and in the bubbles size.

One of the most important parameters regarding the motion of a fuel particle inside the dense bed is the circulation time, defined as the time spent by a fuel particle moving from the bed surface to a determined depth and back to the surface. The circulation time is calculated for both kind of simulations and compared with the experimental results obtained in Soria-Verdugo et al. [6] and Soria-Verdugo et al. [9]. The circulation time is represented in Figure 6 in the form of boxplots for both the experimental and numerical cases, considering the two different fuel densities.

It can be observed in Figure 6 that the simulation accounting for the wall friction represents with good agreement the circulation time of a fuel particle, not only in terms of the median values obtained, but also in terms of the statistical distribution. In view of the results, it can be concluded that the influence of the wall friction term in the simulation of the motion of a fuel particle in a pseudo-2D bed is significant. In the case of not considering wall friction, a substantial sub-estimation of the circulation time is observed for the two fuel particle densities under study. This result is in agreement with the rising and sinking velocities shown in Figure 5 and with the number of jumps presented in Figure 4. Higher ascending and descending velocities of the fuel particle imply lower circulation times in the dense bed, with a similar number of jumps for each cycle. Regarding the influence of the density of the fuel particle on the circulation time, no substantial differences can be found in the experiments or the simulations for the low densities variations considered. This similitude can be attributed to the concordance in the motion of the fuel particle for these two densities, as Soria-Verdugo et al. [9] described. A proper circulation of the fuel particle in the whole bed, together with

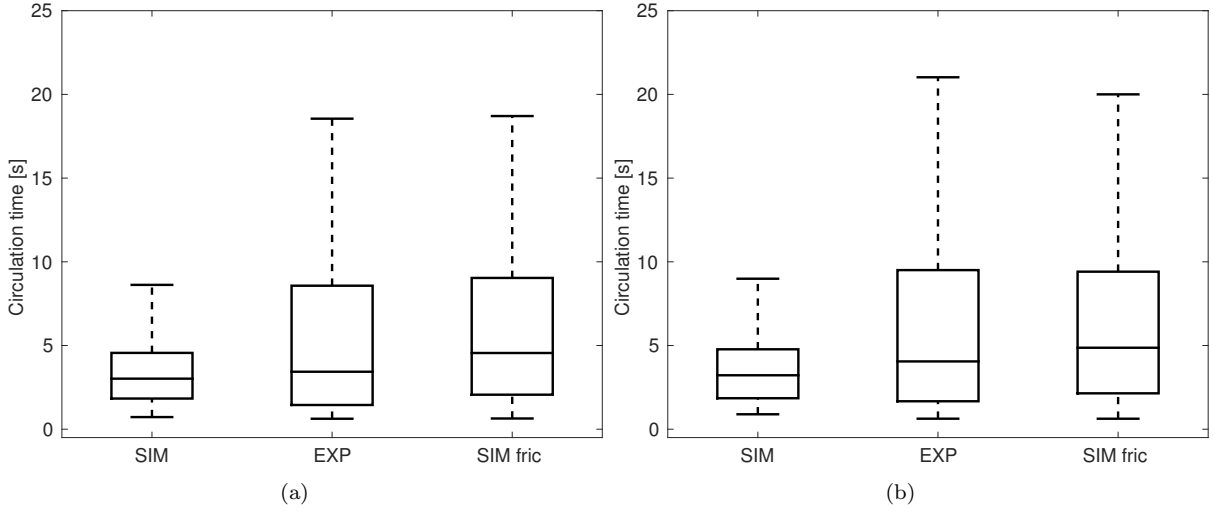


Figure 6: Circulation time spent by the fuel particle in a cycle. a) Flotsam fuel particle. b) Neutrally fuel particle.

the analogous velocities obtained during the rising and sinking processes promote a very similar circulation time. Nevertheless, higher variations of the fuel particles density might influence the circulation times both in the experiments and the simulations.

Table 4 presents the percentage of time spent by the fuel particle at the freeboard, P_{fb} , and inside the dense bed, P_{db} , for the different cases studied. P_{fb} is defined as the ratio between the time that the fuel particle is at the freeboard, i.e. at a height over the average bed surface height, \bar{h}_{fb} , and the total sampled time. On the other hand, P_{db} is calculated as the ratio between the time that fuel particle is inside the dense bed, i.e. below \bar{h}_{fb} , and the total sampled time. The results of Table 4 show the buoyant effect of the different fuel particles, obtaining a higher time spent by the flotsam particle at the freeboard in comparison to that of the neutrally buoyant particle. This results represents the larger buoyancy of the less dense particle in both simulations and in the experiments. Furthermore, the results of the simulation considering the friction term are in very good agreement with the experimental results, in contrast with the results of the simulation neglecting the friction term, where the time spent by the fuel particle in the freeboard is larger. This fact is in accordance with the results showed previously and are attributed to the higher coalescence of bubbles and the diminution of the height of the bed surface when the wall friction term is neglected in the simulation.

Table 4: Percentage of the time that the fuel particle is located in the freeboard and inside the bed for the different cases studied.

	\bar{h}_{fb} [cm]	Flotsam particle		Neutrally buoyant particle	
		P_{fb} [%]	P_{db} [%]	P_{fb} [%]	P_{db} [%]
EXP	61.5	9	91	6.9	93.1
SIM fric	61.5	8.1	91.9	7	93
SIM	58.5	16.3	83.7	11.6	88.4

4. Conclusions

The motion of a fuel particle in a pseudo-2D bubbling fluidized bed was simulated using a hybrid TFM-DEM model in combination with a friction term that accounts for the effect of the front and rear walls of the bed vessel, as proposed by Hernández-Jiménez et al. [31]. The simulation results were compared with the experimental evidence obtained by Soria-Verdugo et al. [6, 9].

Considering the motion of the fuel particle in the bed, both kind of simulations, with and without considering the friction term, show a reasonable good agreement with the experimental data as far as the location of the fuel particle is concerned. The relative frequency of finding the fuel particle at a certain bed height and the experimental fitting of the geometrical law used to determine the number of jumps needed by the fuel particle to reach the bed surface are well predicted by the simulations. However, it was found that the simulation without the friction term predicts a lower number of jumps than the experiments, for both fuel densities analyzed. The numerical prediction of the number of jumps matches the experimental findings when the friction term is incorporated in the simulation.

Regarding the mean fuel particle velocity for both the sinking and the rising processes, the simulation results without the friction term presents values more than the double of the experimental findings. Concerning the circulation time spent by the fuel particle in a cycle, only the simulation with the friction term is capable of reproducing both the median values and the shape of the experimentally measured probability density function of the circulation time.

In summary, the present work shows the capability of the hybrid TFM-DEM model to reproduce the motion of fuel particles in a pseudo-2D fluidized bed when the effect of the front and rear walls is considered. This practical validation confirms the possibility of using the TFM-DEM model to reproduce the motion of fuel particles in medium or large scale facilities not only in 3D systems, but in systems in which the bed walls are playing an important role.

Nomenclature

C_{sp}	Coefficient of friction between unlike solids [-]
c	Particle–wall interaction coefficient [kg/m ² s]
D_b	Bubble diameter [m]
d_p	Discrete particle diameter [m]
d_s	Dense phase particle diameter [m]
e_{sp}	Coefficient of restitution [-]
\vec{F}_c	Net contact force on each discrete particle [N]
\vec{F}_d	Total gas–solid drag force on each discrete particle [N]
\vec{F}_T	Net sum of all forces on each discrete particle [N]
\vec{f}_{fric}	Frictional force per unit volume [N/m ³]
\vec{g}	Gravity [m ² /s]
$g_{0,sp}$	Radial distribution function at contact [-]
H	Bed height [m]
h_0	Static bed height [m]
h_{fb}	The average bed height [m]
I	Moment of inertia [kg m ²]
\bar{I}	Unity matrix [-]
K_{gs}	Drag force between gas and solids [kg/m ³ s]
K_{pg}	Drag force between discrete particle and gas [kg/m ³ s]
K_{ps}	Drag force between discrete particle and solids [kg/m ³ s]
k_{Θ}	Diffusion coefficient for granular energy [kg/ms]
m	Mass [kg]
N_j	Number of jumps [-]
P_{N_j}	Relative frequency of the number of jumps needed by a fuel particle to reach the bed surface [-]

P_{db}	Percentage of time that the fuel particle is located inside the bed [%]
P_{fb}	Percentage of time that the fuel particle is located at the freeboard [%]
p	Geometrical fitting parameter of the number of jumps [-]
p_g	Gas pressure [Pa]
p_s	Solids pressure [Pa]
\vec{T}	Net torque acting on each discrete particle [N m]
t	Time [s]
U/U_{mf}	Dimensionless gas superficial velocity [-]
U_{mf}	Minimum fluidization velocity [m/s]
\vec{V}	Velocity vector for discrete particles [m/s]
\vec{v}_g	Gas velocity in each computational cell of the TFM [m/s]
\vec{v}_p	Discrete particle velocity [m/s]
\vec{v}_s	Solids velocity in each computational cell of the TFM [m/s]
W	Bed width [m]
\vec{X}	Position vector for discrete particles [m]
x	Horizontal coordinate [m]
y	Vertical coordinate [m]
Z	Bed thickness [m]

Greek letters

α_g	Gas volume fraction [-]
α_s	Solids volume fraction [-]
Δs	Grid size in the computational domain [m]
γ_Θ	Collisional dissipation of Θ [m ² /s ²]
λ_i	Bulk viscosity [Pa s]

μ_g	Gas viscosity [Pa s]
μ_s	Solids viscosity [Pa s]
$\bar{\alpha}_s$	Normalized solids volume fraction [–]
$\bar{\bar{\tau}}_g$	Gas stress tensor [Pa]
$\bar{\bar{\tau}}_s$	Solids stress tensor [Pa]
Φ	Angle of internal friction [deg]
ρ_b	Bulk density of the bed [kg/m ³]
ρ_g	Gas density [kg/m ³]
ρ_p	Discrete particle density [kg/m ³]
ρ_s	Dense phase particle density [kg/m ³]
Θ	Granular temperature [m ² /s ²]
$\vec{\omega}$	Angular velocity [rad/s]

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References

- [1] D. Kunii, O. Levenspiel, *Fluidization Engineering*, 2nd ed., Butterworth-Heinemann, Boston, 1991.
- [2] A. Gómez-Barea, B. Leckner, Modeling of biomass gasification in fluidized bed, *Prog. Energ. Combust.* 36 (2010) 444–509.
- [3] A. Nienow, P. Rowe, T. Chiba, Mixing and segregation of a small portion of large particles in gas fluidized beds of considerably smaller ones, *AIChE Symposium Series 74* (1978) 45–53.
- [4] K. Lim, P. Agarwal, Circulatory motion of a large and lighter sphere in a bubbling fluidized bed of smaller and heavier particles, *Chemical Engineering Science* 49 (1994) 421–424.
- [5] D. Pallarès, F. Johnsson, A novel technique for particle tracking in cold 2-dimensional fluidized beds simulating fuel dispersion, *Chemical Engineering Science* 61 (2006) 2710–2720.
- [6] A. Soria-Verdugo, L. M. Garcia-Gutierrez, S. Sánchez-Delgado, U. Ruiz-Rivas, Circulation of an object immersed in a bubbling fluidized bed, *Chemical Engineering Science* 66 (2011) 78–87.
- [7] F. Fotovat, J. Chaouki, Characterization of the upward motion of an object immersed in a bubbling fluidized bed of fine particles, *Chemical Engineering Journal* 280 (2015) 26 – 35.
- [8] G. M. Rios, K. Dang Tran, H. Masson, Free object motion in a gas fluidized bed, *Chemical Engineering Communications* 47 (1986) 247–272.

- [9] A. Soria-Verdugo, L. M. Garcia-Gutierrez, N. García-Hernando, U. Ruiz-Rivas, Buoyancy effects on objects moving in a bubbling fluidized bed, *Chemical Engineering Science* 66 (2011) 2833 – 2841.
- [10] A. Soria-Verdugo, N. García-Hernando, J. A. Almendros-Ibáñez, U. Ruiz-Rivas, Motion of a large object in a bubbling fluidized bed with a rotating distributor, *Chemical Engineering and Processing: Process Intensification* 50 (2011) 859 – 868.
- [11] L. M. Garcia-Gutierrez, A. Soria-Verdugo, C. Marugán-Cruz, U. Ruiz-Rivas, Simulation and experimental study on the motion of non-reacting objects in the freeboard of a fluidized bed, *Powder Technology* 263 (2014) 112 – 120.
- [12] L. M. Garcia-Gutierrez, A. Soria-Verdugo, N. García-Hernando, U. Ruiz-Rivas, Simulation of object motion in a bubbling fluidized bed using a monte carlo method, *Chemical Engineering Science* 96 (2013) 26–32.
- [13] L. M. Garcia-Gutierrez, A. Soria-Verdugo, U. Ruiz-Rivas, Optimization of the feeding ports location in a fluidized bed combustor based on monte carlo simulations of fuel particles motion, *Fuel* 141 (2015) 82–92.
- [14] J. A. M. Kuipers, K. J. Van Duin, F. P. H. Van Beckum, W. P. M. Van Swaaij, A numerical model of gas-fluidized beds, *Chemical Engineering Science* 47 (1992) 1913 – 1924.
- [15] D. Gidaspow, *Multiphase flow and Fluidization: Continuum and kinetic theory descriptions*, Academic Press, San Diego, CA, 1994.
- [16] B. G. M. van Wachem, A. E. Almstedt, Methods for multiphase computational fluid dynamics, *Chemical Engineering Journal* 96 (2003) 81 – 98.
- [17] N. G. Deen, M. Van Sint Annaland, M. A. Van der Hoef, J. A. M. Kuipers, Review of discrete particle modeling of fluidized beds, *Chemical Engineering Science* 62 (2007) 28 – 44.
- [18] C. R. Müller, D. J. Holland, A. J. Sederman, S. A. Scott, J. S. Dennis, L. F. Gladden, Granular temperature: Comparison of magnetic resonance measurements with discrete element model simulations, *Powder Technology* 184 (2008) 241 – 253.
- [19] F. Hernández-Jiménez, L. M. Garcia-Gutierrez, A. Soria-Verdugo, A. Acosta-Iborra, Fully coupled TFM-DEM simulations to study the motion of fuel particles in a fluidized bed, *Chemical Engineering Science* 134 (2015) 57 – 66.
- [20] J. R. Grace, F. Taghipour, Verification and validation of CFD models and dynamic similarity for fluidized beds, *Powder Technology* 139 (2004) 99 – 110.
- [21] J. R. Grace, T. Li, Complementarity of CFD, experimentation and reactor models for solving challenging fluidization problems, *Particuology* 8 (2010) 498 – 500.
- [22] Q. Wang, Y. Feng, J. Lu, W. Yin, H. Yang, P. Witt, M. Zhang, Numerical study of particle segregation in a coal beneficiation fluidized bed by a TFM-DEM hybrid model: Influence of coal particle size and density, *Chemical Engineering Journal* 260 (2015) 240–257.
- [23] Q. Wang, H. Yang, Y. Feng, P. Witt, J. Lu, W. Yin, L. Qing, L. Wei, Numerical study of the effect of operation parameters on particle segregation in a coal beneficiation fluidized bed by a TFM-DEM hybrid model, *Chemical Engineering Science* 131 (2015) 256–270.
- [24] T. Li, J. R. Grace, X. Bi, Study of wall boundary condition in numerical simulations of bubbling fluidized beds, *Powder Technology* 203 (2010) 447 – 457.
- [25] F. Hernández-Jiménez, J. Sánchez-Prieto, A. Soria-Verdugo, A. Acosta-Iborra, Experimental quantification of the particle-wall frictional forces in pseudo-2D gas fluidised beds, *Chemical Engineering Science* 102 (2013) 257 – 267.
- [26] T. Kawaguchi, T. Tanaka, Y. Tsuji, Numerical simulation of two-dimensional fluidized beds using the discrete element method (comparison between the two- and three-dimensional models), *Powder Technology* 96 (1998) 129 – 138.
- [27] Y. Q. Feng, A. B. Yu, Effect of bed thickness on the segregation behavior of particle mixtures in a gas fluidized bed, *Industrial & Engineering Chemistry Research* 49 (2010) 3459 – 3468.
- [28] T. Li, P. Gopalakrishnan, R. Garg, M. Shahnam, CFD-DEM study of effect of bed thickness for bubbling fluidized beds, *Particuology* 10 (2012) 532 – 541.

- [29] T. Li, Y. Zhang, A new model for two-dimensional numerical simulation of pseudo-2D gas-solids fluidized beds, *Chemical Engineering Science* 102 (2013) 246 – 256.
- [30] F. Hernández-Jiménez, T. Li, E. Cano-Pleite, W. Rogers, A. Acosta-Iborra, Characterization of the particle-wall frictional forces in pseudo-2D fluidized beds using DEM, *Chemical Engineering Science* 116 (2014) 136 – 143.
- [31] F. Hernández-Jiménez, J. Sánchez-Prieto, E. Cano-Pleite, L. M. Garcia-Gutierrez, A. Acosta-Iborra, Development of an empirical wall-friction model for 2D simulations of pseudo-2D bubbling fluidized beds, *Advanced Powder Technology* 27 (2016) 521 – 530.
- [32] M. Syamlal, W. Rogers, T. J. O'Brien, MFIx Documentation: Theory Guide, U.S. Department of Energy (DOE), Morgantown Energy Technology Center, Morgantown, West Virginia, 1993.
- [33] S. Benyahia, M. Syamlal, T. J. O'Brien, Summary of MFIx equations 2005-4, 2007.
- [34] P. Cundall, C. Strack, A discrete numerical-model for granular assemblies, *Geotechnique* 29 (1979) 47 – 65.
- [35] Y. Tsuji, T. Kawaguchi, T. Tanaka, Discrete particle simulation of two-dimensional fluidized bed, *Powder Technology* 77 (1993) 79 – 87.
- [36] M. Syamlal, The particle-particle drag term in a multiparticle model of fluidization, Technical Report, EG and G Washington Analytical Services Center, Inc., 1987.
- [37] J. L. Lebowitz, Exact solution of generalized percus-yevick equation for a mixture of hard spheres, *Phys. Rev.* 133 (1964) A895 – A899.
- [38] S. Karri, J. Werther, *Handbook of fluidization and fluid-particle systems*, Marcel Dekker Inc., New York, 2003.
- [39] F. Hernández-Jiménez, J. Third, A. Acosta-Iborra, C. Müller, Comparison of bubble eruption models with two-fluid simulations in a 2D gas-fluidized bed, *Chemical Engineering Journal* 171 (2011) 328 – 339.
- [40] J. Davidson, D. Harrison, *Fluidised particles*, 1st ed., Cambridge University Press, Cambridge, 1963.