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Fully coupled TFM-DEM simulations to study the motion of fuel particles in a fluidized bed

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Abstract

In the present work, novel numerical simulations using a hybrid model are carried out to study the motion of objects, representing fuel particles, in a pseudo-2D fluidized bed. The hybrid model combines the continuum treatment of the gas phase with the possibility to treat different solids phases either as continuum, or discrete. In the present case, both the gas and the dense phase of the bed are modelled as continuum phases, as typically done in two-fluid model simulations, whereas fuel particles are simulated as discrete entities whose movement affects, and can be affected by the dense phase motion (i.e. fully coupled TFM-DEM simulations). The results obtained from the model are qualitatively and quantitatively compared with reported experimental findings available in the literature. Firstly, the motion of the fuel particle with regards to the bubble phase and dense phase is proved to be realistic. Secondly, the location probability of the particle in the simulated bed is calculated and compared with the experimental data. Then, the ballistic path followed by the particle in the freeboard are also compared with experimental measurements. These results show good agreement between experiments and simulation. The numerical results reflect the same behaviour during the ascending and descending motion of the fuel particles as that observed in the experiments. The results also show that the most probable locations of the particles predicted by the simulations are consistent with the experimental findings, both inside the fluidized bed and in the freeboard. Overall, the hybrid model tested shows quite promising results, which indicates the potential usability of the model.

Keywords: Fluidized bed, Pseudo-2D, Object motion, Fuel particle, Hybrid model, Fully coupled simulation.

1. Introduction

Despite the fact that fluidized beds have been used in industry since the 1920s and great progress has been made, some aspects of fluidized bed dynamics are still far from being fully understood. In particular,
for thermal conversion of solids fuels, the motion and distribution of fuel particles throughout the bed are key points affecting the performance of fluidized bed combustors. The vertical and lateral motions, the residence time in the dense bed, and the chemical conversion of fuel particles are main parameters for the design of fluidized bed reactors (Gómez-Barea and Leckner, 2010).

Concerning the vertical motion of fuel particles in fluidized beds, several authors have studied the rising and sinking process of fuel particles in two-dimensional (2D) and three-dimensional (3D) facilities. During the rising process, the successive passing bubbles lift the particle from inside the dense bed to the bed surface in small paths called jumps (Rios et al., 1986; Soria-Verdugo et al., 2011a). During the sinking process, the particle descends by the lateral sides of the bed following the motion of the dense phase, which increases the residence time of the fuel particle in that part of the bed (Nienow et al., 1978; Kunii and Levenspiel, 1991; Rees et al., 2005; Pallarès and Johnsson, 2006; Soria-Verdugo et al., 2011a). The influence of buoyancy effects on the particle motion and the circulation time of the particle inside the dense bed were experimentally studied by Soria-Verdugo et al. (2011b,c) in 2D and 3D fluidized beds. Later, the motion of fuel particles inside the dense bed in a 2D bubbling fluidized bed was modelled by Garcia-Gutierrez et al. (2013) using a Monte Carlo method. Regarding the lateral motion of a particle in a fluidized bed, it was experimentally studied by Olsson et al. (2012) and Sette et al. (2014) in cold 3D fluidized beds, and modelled by Garcia-Gutierrez et al. (2015) using a statistical model. Furthermore, the residence time and the lateral displacement when the fuel particle is in the freeboard are also key parameters in the thermal conversion process. Garcia-Gutierrez et al. (2014) experimentally characterised the motion of a fuel particle in the freeboard and confirmed that the motion of the particle in the freeboard is ballistic when the bed is operating in bubbling regime.

Most of the previous studies were conducted in pseudo two-dimensional (pseudo-2D) beds, which have been crucial for the understanding of the dynamics of gas–particle systems. See for example Shen et al. (2004); Santana et al. (2005); Almendros-Ibáñez et al. (2006); Müller et al. (2007); Laverman et al. (2008); Busciglio et al. (2008); Sánchez-Delgado et al. (2010); Hernández-Jiménez et al. (2011b); Sánchez-Delgado et al. (2013), where non-intrusive experimental techniques such as Digital Image Analysis (DIA) or Particle Image Velocimetry (PIV) where applied to the images acquired from the front view of the bed.

Another approach to the understanding of fluidized bed performance are numerical simulations. In general, simulations of fluidized beds can be performed using Eulerian-Eulerian Two-Fluid Models (TFM) or Eulerian-Lagrangian approaches such as Discrete Element Models (DEM). These models can be a very effective complementary tool to the experiments for achieving a detailed analysis of hydrodynamics in complex gas-solid flows (Grace and Taghipour, 2004; Grace and Li, 2010). For example, in the last years a few works have used numerical simulations to model fuel mixing in gas–solid fluidized beds. Farzaneh et al. (2011) used a multigrid technique for Lagrangian modeling of fuel particles in a fluidized bed, which improves considerably the results compared to simulations using a single-grid approach. In a recent work, Farzaneh et
al. (2015) combined a Eulerian-Lagrangian and Eulerian-Eulerian frameworks to simulate the behaviour of a limited number of fuel particles in a bubbling gas-solid fluidized bed by employing different frictional stress theories. They concluded that the simulation with a visco-plastic stress model leads to results that are in much better agreement with experiments than those obtained employing others models. It is important to note that in the work by Farzaneh et al. (2015) the solids phase (i.e. bed material) was resolved within the Eulerian TFM framework and the fuel particles were tracked separately using information obtained from the TFM simulation. This means that their simulation of the fuel particles was partially uncoupled with the actual continuum phases, since the gas and dense phases were not influenced by the presence of the fuel particles in the bed.

In the present work, novel numerical simulations using a hybrid model are carried out to study the motion of fuel particles in a cold pseudo-2D fluidized bed unit. This work serves as a first practical validation of the hybrid model, which is an essential step before using the numerical results for the analysis of the motion of fuel particles inside fluidized bed reactors. The hybrid model is a fully coupled TFM-DEM strategy that combines the continuum treatment of the gas phase with the possibility of solving it together with different solids phases either as continuum, or discrete. In the present case, both the gas and the dense phases of the bed are modelled as continuum phases, as typically done in two-fluid model simulations; whereas the fuel particles are considered as discrete inert entities that can also affect the gas and dense phase. The numerical simulations are performed using the MFIX-Hybrid code. In a first step, the results obtained from the model are qualitatively and quantitatively compared with the experimental findings obtained by Soria-Verdugo et al. (2011a) when the particles are inside the dense bed. Then, the results for the particle motion in the freeboard are compared with the experimental data reported by Garcia-Gutierrez et al. (2014). The relation between the motion of the particle, when it is inside the dense bed, and the bubble and dense phases in the simulation results is analysed and compared with the experimental data. Then, the similarity between the preferred paths followed by the fuel particles obtained by both the simulations and the experimental work is discussed. Finally, the particle motion in the freeboard is also extracted from the numerical model and statistically analysed and compared with the experimental results.

2. MFIX-DEM simulations

2.1. Numerical model

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, an Eulerian-Lagrangian-Eulerian approach is employed. The gas phase is treated as continuum, and the different solids 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 modelled 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 (Syamlal et al., 1993; Benyahia et al., 2007). The granular temperature, analogously to the motion of molecules in a gas, is proportional to the mean quadratic difference of the individual velocity of particles and their bulk velocity, \( \Theta = \langle \tilde{v}_{s,ind} - \tilde{v}_s \rangle^2 \rangle / 3 \). Using the kinetic theory of granular flow, the granular temperature appears in the closure of the solids stress and other terms of the governing equations. The closure expressions for the Eulerian-Eulerian model can be found in Benyahia et al. (2007).

In the discrete description of the present study, the fuel particles are represented by actual individual particles in the flow, and inter-particle collisions are directly solved using the soft-sphere approach proposed by Cundall and Strack (1979) and Tsuji et al. (1993). In the soft-sphere approach, the overlap between the two particles is represented as a system of springs and dashpots in both the normal and tangential directions. The spring causes the rebound off the colliding particles and the dashpot mimics the dissipation of kinetic energy due to inelastic collisions. In addition, the gas and dense phases volume fractions in the continuum description are also influenced by the presence of the discrete fuel particles (i.e. fully coupled TFM-DEM). Details of the governing equations along with the numerical implementation, including the coupling procedure, tests and validations, can be found in Garg et al. (2010, 2012) and Li et al. (2012).

The governing equations for the hybrid model are summarised in the following lines. The subscript \( s \) is referred to the solids—continuum phase, \( g \) to the gas phase and \( p \) to the discrete fuel particles.

Mass conservation of the gas and solids phases, continuum:

\[
\frac{\partial}{\partial t} (\alpha_g \rho_g) + \nabla \cdot (\alpha_g \rho_g \tilde{v}_g) = 0
\]

Momentum conservation of the gas and solids phases, continuum:

\[
\frac{\partial}{\partial t} (\alpha_g \rho_g \tilde{v}_g^2) + \nabla \cdot (\alpha_g \rho_g \tilde{v}_g^2) =
\]

\[
-\alpha_g \nabla p + \nabla \cdot \rho_g \tilde{g} + \alpha_g \rho_g \tilde{g} + K_{gs} (\tilde{v}_g^* - \tilde{v}_s^*) + K_{pg} (\tilde{v}_p^* - \tilde{v}_g^*)
\]

\[
\frac{\partial}{\partial t} (\alpha_s \rho_s \tilde{v}_s^2) + \nabla \cdot (\alpha_s \rho_s \tilde{v}_s^2) =
\]

\[
-\alpha_s \nabla p + \nabla \cdot \rho_s \tilde{g} + \alpha_s \rho_s \tilde{g} + K_{gs} (\tilde{v}_g^* - \tilde{v}_s^*) + K_{ps} (\tilde{v}_p^* - \tilde{v}_s^*)
\]
Granular temperature, $\Theta$, balance equation:

$$
\frac{3}{2} \left( \frac{\partial}{\partial t} (p_s \alpha_s \Theta) + \nabla \cdot (p_s \alpha_s \vec{v}_s \Theta) \right) = 
$$

$$
(-p_s \vec{I} + \tau) : \nabla \vec{v}_s + \nabla \cdot (k_\Theta \nabla \Theta) - \gamma_\Theta - 3K_{gs} \Theta
$$

where $p_s$ is the solids pressure, $\tau_i$ is the strain tensor for phase $i$, $((-p_s \vec{I} + \tau) : \nabla \vec{v}_s)$ is the generation of $\Theta$ by the solids stresses, $k_\Theta \nabla \Theta$ accounts for the diffusion of $\Theta$, $\gamma_\Theta$ is the collisional dissipation of $\Theta$ and $3K_{gs} \Theta$ is the transfer of random kinetic energy between the solids and the gas. In the above equations $K_{gs}$ and $K_{ps}$ are the drag force coefficients between the gas and the solids phases, and between the discrete particles and the solids phase, respectively. The contribution of $K_{ps}$ in the granular temperature balance equation is ignored in this work.

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:

$$
\frac{d\vec{X}_j}{dt} = \vec{V}_j
$$

$$
m^j \frac{d\vec{V}_j}{dt} = \vec{F}_j^d = m^j \vec{g} + \vec{F}_j^c + \vec{F}_j^i
$$

$$
P^j \frac{d\vec{\omega}_j}{dt} = \vec{T}_j
$$

where $m^j$ and $I^j$ are the mass and moment of inertia of each $j$ particle, $\vec{F}_j^d$ is the net contact force on a particle as a result of contact with other discrete particles. $\vec{F}_j^c$ also includes the net force produced by the collisions of the solids phase on the discrete particles given by $K_{ps}(\vec{v}_s - \vec{v}_p)$, $\vec{F}_j^d$ is the total gas–solid drag force (pressure and viscous) on each particle $j$ produced by the solids phase (bed material), and $\vec{F}_j^i$ 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 solids particles (continuum or dense) or walls.

The drag force correlation for all the gas–solid interaction, $K_{gs}$ and $K_{pg}$, is selected as the one proposed by Gidaspow (1994). For the particle–solids phase interaction, the coefficient $K_{ps}$ derived by Syamlal (1987) as a simplified version of kinetic theory is used in the present simulations:

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

where $e_{sp}$ and $C_{sp}$ are the coefficients of restitution and friction, respectively, between the solids phase and the discrete particles. The radial distribution function at contact, $g_{0,sp}$, was that derived by Lebowitz
(1964) for a mixture of hard spheres of different sizes:

\[
g_{0,sp} = \frac{1}{\alpha_g} + \frac{3d_p d_s}{\alpha_g^2 (d_p + d_s)} \sum_{\lambda=1}^{M} \frac{a_{s\lambda}}{d_{p\lambda}}
\]

where \(\lambda\) goes from 1 to \(M\), being \(M\) the total number of solids phases, discrete and continuum.

2.2. Simulated system

The simulated system employed in this work was chosen to match the experimental set-up tested by Soria-Verdugo et al. (2011a). The experimental system is a pseudo-2D cold fluidized bed of dimensions 0.5 m x 1.5 m x 0.01 m (width \(W\), height \(H\), and thickness \(Z\)). Since the motion is practically restricted to the horizontal and vertical directions, the simulation only covers these two dimensions, i.e. 2D domain (0.5 m x 1.5 m). The simulated bed material was spherical particles of 2500 kg/m\(^3\) density and average particle diameter of 0.7 mm, which correspond to the medium size and density of the bed material used by Soria-Verdugo et al. (2011a). A summary of the numerical parameters employed is included in Tables 1 and 2. It is important to remark that the gas and dense phases (bed material) are described as continuum phases whereas the fuel particles are simulated as discrete entities. The properties of the discrete particles are chosen to match the experimental data reported by Soria-Verdugo et al. (2011a). In particular, the shape of the particles is simplified to circular particles with an equivalent diameter that accounts for the same mass as the cylindrical pellets tested in the experiments (Table 2). Instead of a single fuel particle emulating the individual particle tracked in the experimental procedure, three identical particles are simulated to obtain more representative statistical data while guaranteeing a negligible interaction between them. The number of collisions recorded is below 0.02 per second. The selection of the simulation properties for the discrete particles is made to reduce the effect of their collisions with other discrete particles on the motion of the dense phase. The static bed height was 0.5 m both in the experiments and simulations. The solids continuum phase of the simulation is similar to the bed material from the experiments. The superficial gas velocity is 2.5\(U_{mf}\) as in Soria-Verdugo et al. (2011a) ensuring a bubbling regime. The pressure drop along the distributor in the experimental facility corresponds to a 61% of the bed pressure drop for the operating conditions studied in the present work. This ensures that the bed and the air supply system were independent and a uniform air inlet along the width of the bed is guaranteed. Details about the experimental distributor design and characterisation can be found in Soria-Verdugo et al. (2011a). The 2D computational domain is discretised by a uniform grid with cells of \(\Delta s = 5\) mm size in horizontal and vertical directions (100 x 300 cells). Gas flow is fed uniformly at the bottom of the bed using a velocity inlet boundary condition, which represents an air supply system independent from the bed (i.e. large distributor-to-bed pressure ratio). The gas flow then leaves the system through the top boundary at a constant pressure. A no-slip boundary condition is used for the gas and continuum solids phases at the side walls of the bed. It has been previously shown
that the lateral boundary condition does not have a strong effect in this kind of simulations (Li et al., 2010; Hernández-Jiménez et al., 2011a).

It is worth to mention that the time step for the solution procedure must be limited in this kind of simulations to accurately solve the interaction between the continuum phases and the discrete fuel particles. Thus, the time step is reduced around 10 times compared to a typical two-fluid model simulation of a similar bed without discrete particles. This, in combination with the long time needed to have enough statistical data, forces the simulation to be as simpler as possible to facilitate the study.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bed height, $H$ (m)</td>
<td>1.5</td>
</tr>
<tr>
<td>Bed width, $W$ (m)</td>
<td>0.5</td>
</tr>
<tr>
<td>Static bed height, $h_0$ (m)</td>
<td>0.5</td>
</tr>
<tr>
<td>Particles density, $\rho_s$ (kg/m$^3$)</td>
<td>2500</td>
</tr>
<tr>
<td>Particle diameter, $d_s$ (mm)</td>
<td>0.7</td>
</tr>
<tr>
<td>Gas density, $\rho_g$ (kg/m$^3$)</td>
<td>1.2</td>
</tr>
<tr>
<td>Coefficient of restitution, $e_s = e_{sp}$ (−)</td>
<td>0.9</td>
</tr>
<tr>
<td>Angle of internal friction, $\Phi$ (deg)</td>
<td>30</td>
</tr>
</tbody>
</table>

Table 2: Simulation parameters for discrete fuel particles.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particles density, $\rho_p$ (kg/m$^3$)</td>
<td>1580</td>
</tr>
<tr>
<td>Particle diameter, $d_p$ (cm)</td>
<td>1.06</td>
</tr>
<tr>
<td>Normal inter-particle spring constant (N/m)</td>
<td>1000</td>
</tr>
<tr>
<td>Tangential inter-particle spring constant (N/m)</td>
<td>286</td>
</tr>
<tr>
<td>Normal wall-particle spring constant (N/m)</td>
<td>1000</td>
</tr>
<tr>
<td>Tangential wall-particle spring constant (N/m)</td>
<td>286</td>
</tr>
<tr>
<td>Particle-particle friction coefficient (−)</td>
<td>0.0</td>
</tr>
<tr>
<td>Particle-wall friction coefficient (−)</td>
<td>0.0</td>
</tr>
<tr>
<td>Particle-particle restitution coefficient (−)</td>
<td>0.0</td>
</tr>
<tr>
<td>Particle-wall restitution coefficient (−)</td>
<td>0.0</td>
</tr>
<tr>
<td>Coefficient of friction between unlike solids, $C_{sp}$ (−)</td>
<td>0.1</td>
</tr>
</tbody>
</table>

The simulation is started with the bed material resting in the lower part of the bed. The discrete particles are initially placed just on the surface of the bed. Figure 1a presents the solids volume fraction at the initial time step, together with the discrete fuel particles represented as black points. Note that the size of the discrete particles is exaggerated in Figure 1 to enhance visualisation. The total simulated time was 240 seconds, and considering the three particles simulated it makes 720 seconds of simulated data. Once the simulation commences, bubbles appear mixing the bed material and distributing the fuel particles within the bed. Figure 1b shows a snapshot of the solids volume fraction with fuel particles after 15 seconds of simulated time.
Figure 1: Solids volume fraction $\alpha_s$ at the initial time step (a) and after 15 seconds of simulated time (b), with the discrete fuel particles represented as black points. Note that the representation of the fuel particles is exaggerated to enhance visualisation.

3. Results

The results section is divided in two main parts. The first part focuses on analysing the behaviour of the fuel particle inside the dense bed in the simulations, and comparing with the experimental results from Soria-Verdugo et al. (2011a). The second part focuses on the fuel particle motion in the freeboard with the aim of verifying whether the simulated particle follows a ballistic path and whether this particle path in the freeboard is analogous to the experimental data obtained by Garcia-Gutierrez et al. (2014).

3.1. Fuel particle motion inside the dense bed

As stated in the Introduction section, fuel particles tend to descend by the sides of the bed and ascend in the middle of the bed provided that there is a single bubble path in the centre of the bed. On the other hand, if more preferred bubble paths appear in the bed, the solids will additionally descend between the different bubble paths, as reported by Pallarès and Johnsson (2006). Moreover, in the rising process, a fuel particle can rise to the bed surface by the action of several passing bubbles, alternating partial rising paths with sinking motions.

In order to evaluate the results of the simulation about the trajectories of the discrete fuel particle in the rising and sinking process, the results were compared with experimental data obtained by Soria-Verdugo et al. (2011a). Figure 2 shows some snapshots at sequential instants of the fuel particle positions in the sinking and rising processes. An example of the fuel particle trajectory obtained by Soria-Verdugo et al. (2011a) in
their experiments is shown in Figure 2a, and an example of the trajectory obtained by the simulation is also illustrated in Figure 2b. In both Figures the particle is marked with a black cross and a black line is used to mark its path.

The sinking path of the fuel particle measured in the experiments is located on the side of the bed, as can be observed in Figure 2a. After that, the particle in the experiments starts a rising path caused by the ascension of a bubble. Nevertheless, the fuel particle does not reach the bed surface in this stage by the action of this single bubble and it sinks again until another bubble appears and pushes the fuel particle up. The simulation is capable of reproducing this rising and sinking behaviour, as can be seen in Figure 2b. Initially (first snapshot in the left of Figure 2b), the simulated fuel particle sinks also by the side of the bed, similarly to the experiments. Then, a passing bubble lifts the fuel particle preventing it to reach the bottom of the simulated bed. At a certain instant, the particle detaches from the bubble starting a new sinking path. Finally, the particle is raised again by the action of another passing bubble (last snapshot of Figure 2b). Figure 2 is an illustration of the rising and sinking processes of the fuel particle inside the dense bed, but it is worth to remark that such processes are repeated continuously during the simulation and the
Some differences between the trajectory of the fuel particle obtained in the experiments and the simulations can be observed in Figure 2. Nevertheless, as commented before the simulation is able to reproduce the sinking process by the sides of the bed and the rising process through the middle. Moreover, the simulation is capable to mimic the phenomenon of small jumps observed in the experiments due to passing bubbles during the rising process (Rios et al., 1986; Soria-Verdugo et al., 2011a). This phenomenon is quantified in Figure 3, where the relative frequency of finding a number of jumps in a cycle is plotted. A cycle is defined as the interval between the instant an object sinks into the bed from its surface and the instant it returns to the surface of the bed. Circles represent the data obtained directly from the simulation, the blue dash line is the geometrical fitting of the simulation data and the black line is the geometrical fitting obtained by Soria-Verdugo et al. (2011a) from the experimental results. The geometrical fitting corresponds to the following equation: \( P(N) = p_j(1 - p_j)^{N-1} \), where \( P \) is the relative frequency of finding a number of jumps in a cycle, \( N \) is the number of jumps in a cycle and \( p_j \) represents the probability of an object to reach the bed surface in one jump when a rising process is started. In the experimental data, the value for \( p_j \) was 0.45 (Soria-Verdugo et al., 2011a,b) whereas for the simulation results \( p_j \) is 0.52.

Quite good agreement is found in the value of \( p_j \) and it can be seen that the numerical results also follow a geometrical distribution, despite the number of cycles extracted from the simulation (196 cycles) is very low compared to the experimental work by Soria-Verdugo et al. (2011a) (over 1200 cycles). Furthermore, the discrepancies between the numerical and experimental data is comparable to the results obtained by (Soria-Verdugo et al., 2011b) for particles of different size and density. Therefore, the fuel particle motion
throughout the bed can be described using the fully coupled TFM-DEM simulations.

Figure 4 shows the relative frequency, $F_R$, of finding the center of mass of the fuel particle at a certain position inside the dense bed. $F_R$ is calculated using sampling cells of 0.05 x 0.05 m$^2$ in all the bed frontal area, for both the simulation (Figure 4a) and experimental results (Figure 4b). The relative frequency at each sampling cell was calculated as the number of instantaneous frames in which the center of mass of the fuel particle was present at that cell, divided by the total number of instantaneous frames. In the case of the simulation, since three discrete fuel particles are in the bed, this result is also divided by the number of particles. Therefore, a higher relative frequency will be obtained in zones where the fuel particle moves with a lower velocity.

The main circulation pattern of the particle is correctly reproduced by the simulation results when compared with experiments (Figure 4). This pattern reflects a fast ascending path in the centre of the bed (values of low relative frequency, $F_R$) and a slow descending motion close to the walls (values of high $F_R$). Nevertheless, certain discrepancies can also be detected. In the simulation results the descending path is closer to the walls and located at lower positions than in the experimental results. These discrepancies can be attributed to two different causes. The first one is related to the modelling of the distributor plate, which consists of a perforated plate in the experimental system, but it is modelled as a uniform velocity inlet in the simulations. Mesh limitations make difficult the discretization of the holes of the experimental distributor and the uniform velocity inlet chosen for the boundary condition is generally accepted as a good approximation. In the simulated distributor, since the gas is entering equally along the whole width of the bed, bubbles are created uniformly and this confines the descending area for the particle to a region very
close to the wall. The second main cause of this discrepancy between the relative frequency obtained from
the experiment and the simulation is related with the number of statistical data used to construct Figure 4.
The experimental data cover 10,000 seconds of fluidized bed activity, whereas the simulated time goes up to
around 700 seconds. Despite of the fact that the simulation time is long, it is still far from the sampling time
achieved in the experimental campaign. The experience gained from experiments indicates that the number
of statistical data needed to study the particle position in a map, such as that represented in Figure 4, is
high. For example, the time needed to reach a stable value of relative frequency is around 5000 s. Beyond
this value the variations of the relative frequency are below 10%. In any case, the results obtained from the
comparison between the experiments and the hybrid TFM-DEM simulation are quite promising.

To perform a more quantitative comparison between numerical and experimental results, Figure 5 shows
the relative frequency, \( F_R \), of rising and sinking particles as a function of bed width. In this figure, \( F_R \)
is the accumulation of the relative frequency for all the positions along the entire height of the bed. The
relative frequency is calculated for both the experimental and simulation data using a width interval of 1
cm. The preferential paths for the sinking and rising motions show a good agreement between experimental
and simulation results. The biggest discrepancies appear in the descending path close to the lateral walls.
These discrepancies were also observed in Figure 4 and, as commented previously, they may be originated
by the distributor modelling and the different amount of data in the simulations and the experiments.

The relative frequency, \( F_R \), to find particles at each vertical position (height above the distributor) is of
prime importance to characterize the particle circulation, since it is an indicator of the capability of the bed
to produce a homogeneous axial mixing of the fuel particles (Soria-Verdugo et al., 2011a). Figure 6 shows
the relative frequency of finding a particle as a function of the vertical position, obtained from both the

![Figure 5: Relative frequency to find a rising and sinking fuel particle as a function of the horizontal position of the bed for the experimental (Soria-Verdugo et al., 2011a) and hybrid TFM-DEM simulation results.](image-url)
experiments and the hybrid TFM-DEM simulation data. The relative frequency is calculated using a height interval of 1 cm. In this case, also good agreement is observed between the experimental and simulation data. Figure 6 shows that the higher probability of finding the fuel particle is located inside the dense bed. The relative frequency grows up to a height shorter than the static bed height, drastically descending for higher heights. This result guarantees a homogeneous distribution of the fuel particles in the vertical direction, achieved for both the experimental and the hybrid TFM-DEM simulation results.

It is worth recalling that the simulations were performed in a 2D domain, which means that the interaction with the front and rear walls is not included. Previous works have shown how these walls affect the dense phase motion in the simulation of pseudo-2D beds (Li et al., 2010; Hernández-Jiménez et al., 2011a; Li and Zang, 2013; Hernández-Jiménez et al., 2013, 2014). Nevertheless, the preliminary comparison performed here is aimed to study the basic interaction between the fuel particle and the dense and bubble phases, without taking into consideration other interactions such as particle or dense phase wall interactions. As stated above, the comparison of the experimental observations with simulation results obtained using the hybrid TFM-DEM model has shown very promising results, but further work is needed to study the importance of the possible effect of the front and rear walls on the motion of fuel particles. Besides, the fuel particles simulated in this work are considered as non-reactive, similarly to the experimental work (Soria-Verdugo et al., 2011a). For reactive fuel particles, it is expected that endogenous bubbles are created by the fuel released gas (Fiorentino et al., 1997a,b). Therefore the motion of reactive fuel particles can be affected by complex two-way interactions between discrete and continuous phases, revealing the importance of a fully coupled simulation of the three phases. Thus, the fully coupled hybrid model employed here will facilitate further studies considering reacting particles.
3.2. Fuel particle motion in the freeboard

In this part of the results, the fuel particle motion in the freeboard described by the simulation is compared with the experimental results reported by Garcia-Gutierrez et al. (2014), who employed a bed similar to Soria-Verdugo et al. (2011a) but with a reduced bed thickness (0.5 cm). This allows the use of the same simulated system of section 3.1. The particle motion in the freeboard is characterized by a ballistic path affected only by gravity. Garcia-Gutierrez et al. (2014) statistically characterized the time of flight and the lateral displacement of the particle during the ballistic path, and developed a model capable of predicting the motion of the fuel particle in freeboard.

In order to analyse the ballistic behaviour of the particle in the simulation results, the same methodology described by Garcia-Gutierrez et al. (2014) was employed. An example of the ballistic behaviour of the fuel particle in the freeboard is plotted in Figure 7a and 7b for the experiments and the simulations, respectively. The vertical coordinate of the particle during the time spent in the freeboard is plotted together with a parabolic fitting. The initial and final instants of the ballistic path are also marked in the figures. The number of ballistic paths obtained in the simulation was 71, which is similar to the number obtained by Garcia-Gutierrez et al. (2014) experimentally (92) and enough to perform a statistical analysis (Garcia-Gutierrez, 2014). In both figures only one ballistic path is depicted as an example. Both the experimental and the simulation data fit quite well with a ballistic path, which reflects the consistency of the simulation results with the experimental measurements, as can be seen in Figure 7.

The lateral displacement, \( \Delta x \), and the maximum height, \( y_{max} \), reached by the fuel particle were obtained in the numerical model by analysing the ballistic paths followed by the fuel particle. The lateral displacement corresponds to the horizontal distance covered by the fuel particle between the final and initial point of the
ballistic path (points marked with a cross in Figure 8a). The maximum height is the maximum vertical position reached by the fuel particle during its ballistic path (Figure 8b). The simulation results are plotted in the form of a box plot together with the experimental results. Box plots include the median value, represented by a horizontal red line, the quartiles corresponding with 25% and 75% of the population, associated to the down and upper horizontal blue lines respectively, a confidence interval delimited with the horizontal black line and the outliers, marked with a ‘+’.

Overall, the simulation results obtained concerning the lateral displacement and the maximum height reached by the fuel particles are of the same order as the results obtained in the experiments. In particular, the lateral displacement, $\Delta x$, shows a similar tendency in the experiment and the simulation, indicating that in most of the ballistic paths, the median values of the lateral displacement is deviated towards lower values, whereas the larger values are quite scattered (Figure 8a). Regarding the maximum height reached by the fuel particles, $y_{\text{max}}$, the tendency is also well predicted by the simulation results, with very similar values for the interquartile range and the upper confidence interval (Figure 8b). It can be concluded that the simulations can predict the trajectory of the fuel particle in the freeboard with reasonably accuracy. Therefore, the hybrid model seems to be a useful tool to predict the fuel particle motion in the freeboard of a reactor.

4. Conclusions

Visual inspection of the results of the Hybrid DEM-TFM simulation analysed in this work showed that the trajectory of the fuel particle inside the dense bed is qualitatively similar to the experimental data, including the sinking path of the fuel particles at the sides of the bed, and the rising path when the fuel
particle is lifted towards the bed surface by several passing bubbles at the centre of the bed. The relative frequency of finding a number of jumps in a cycle was quantified showing quite good agreement between numerical and experimental data. A quantitative analysis was performed through the relative frequency of finding the fuel particle at certain positions and the relative frequency of finding rising and sinking fuel particles. The results showed good agreement between the experimental and simulation data, with some discrepancies in the probability maps in the region close to the lateral walls. The fuel particle motion in the freeboard determined by the simulations represents quite good consistency with experiments. The numerical results showed an analogous tendency to the experimental results concerning the lateral displacement and the maximum height attained by the fuel particles. Furthermore, similar median values of the maximum height reached by the fuel particle are obtained between experiments and simulation. However, further work is needed to fully validate the model, for example by studying the velocity of the fuel particle. Overall, the hybrid TFM-DEM model shows quite promising results that indicate the great potential of the model to be used as an effective complementary tool for the design and optimization of fluidized bed reactors.

**Nomenclature**

\[d = \text{diameter (mm)}\]
\[C = \text{coefficient of friction (-)}\]
\[\epsilon = \text{coefficient of restitution (-)}\]
\[F_c^\text{\text{\tiny net contact force on each discrete particle (N)}}\]
\[F_d^\text{\text{\tiny total gas-solid drag force on each discrete particle (N)}}\]
\[F_R^\text{\text{\tiny relative passing frequency (%)}}\]
\[F_T^\text{\text{\tiny net sum of all forces on each discrete particle (N)}}\]
\[\vec{g} = \text{gravity vector (m/s}^2\text{)}\]
\[g_{\text{sp}} = \text{radial distribution function at contact (-)}\]
\[H = \text{bed height (m)}\]
\[h_0 = \text{static bed height (m)}\]
\[I = \text{moment of inertia of discrete particles (kg m}^2\text{)}\]
\[\mathbb{I} = \text{unity matrix (-)}\]
\[K = \text{drag force between different phases (kg/(m}^3\text{s)})\]
\[k_\Theta = \text{diffusion coefficient for granular energy (kg/(m}^2\text{s))}\]
\[m = \text{discrete particles mass (kg)}\]
\[N = \text{number of jumps in a cycle (-)}\]
\[P = \text{relative frequency of finding a number of jumps in a cycle (-)}\]
\[p = \text{pressure (Pa)}\]
\( p_j \) = probability of an object to reach the bed surface in one jump when a rising process is started (–)

\( \bar{T} \) = net torque acting on each discrete particle (N m)

\( t \) = time (s)

\( U_{mf} \) = minimum fluidization velocity (m/s)

\( \bar{v} \) = velocity vector for the continuum phases (m/s)

\( \bar{V} \) = velocity vector for discrete particles (m/s)

\( W \) = bed width (m)

\( x \) = horizontal coordinate (cm)

\( \bar{X} \) = position vector for discrete particles (m)

\( y \) = vertical coordinate (cm)

\( y_{max} \) = maximum height reached by the particle (cm)

\( Z \) = bed thickness (m)

**Greek letters**

\( \alpha \) = volume fraction (–)

\( \Delta s \) = cell size (mm)

\( \Delta x \) = lateral displacement (cm)

\( \gamma_\Theta \) = collisional dissipation of \( \Theta \) (m\(^2\)/s\(^2\))

\( \Phi \) = angle of internal friction (deg)

\( \rho \) = density (kg/m\(^3\))

\( \bar{\pi} \) = strain tensor (Pa)

\( \Theta \) = granular temperature (m\(^2\)/s\(^2\))

\( \bar{\omega} \) = angular velocity vector for discrete particles (rad/s)

**Subscripts**

\( g \) = gas phase

\( ing \) = individual particle

\( p \) = solid discrete particle

\( s \) = solids continuum phase

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