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OPTIMIZATION OF THE FEEDING PORTS LOCATION IN A FLUIDIZED BED COMBUSTOR BASED ON MONTE CARLO SIMULATIONS OF FUEL PARTICLES MOTION

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Abstract

A Monte Carlo model was proposed to characterize the fuel particles motion in a large-scale fluidized bed. The model describes the global motion of a fuel particle with a proper circulation throughout the bed, analyzing its behavior both in the freeboard and inside the bed. The model was validated with experimental results of the lateral mixing of fuel particles in a large-scale fluidized bed reported in the literature. The lateral displacement of the fuel particles and the residence time, both in the freeboard and inside the bed, were obtained from the model. From those data the lateral dispersion coefficient of the fuel particle was determined. The influence of the operational conditions on the lateral dispersion coefficient and on the maximum lateral distance reached by a fuel particle for different residence times in the bed was also analyzed. Finally, an optimal distance between feeding ports to ensure suitable fuel dispersion was obtained.

Keywords: 3D fluidized bed, Monte Carlo, Fuel particle, Lateral dispersion coefficient, Residence time, Lateral mixing.

1. Introduction

The efficiency of the thermal conversion of solid fuels depends strongly on the characteristics of the technology employed. High volumetric transfer area, homogeneous

temperature, and high mixing rate, make fluidized bed reactors optimal for the chemical transformation of solid fuels. The motion and distribution of fuel particles throughout the bed are key points for the performance of fluidized bed combustors. The lateral and vertical motion, the residence time in the bed, and the chemical conversion of fuel particles are main parameters for the design of fluidized bed reactors [1].

The motion of large objects in a fluidized bed has been studied by several authors for 2D and 3D beds. The sinking and rising processes of an object was described by [2]-[4] showing a good agreement between the object velocity in the sinking process and the downwards velocity of the dense phase material. In the rising process, the object velocity was correlated with a fraction of the bubble velocity, varying between 10 and 30%. The vertical motion of an object in the rising path was associated with a passing bubble, but the object not always reaches the surface of the bed by the action of a single bubble. Rios et al. [5] described the rising process of large objects as a combination of several smaller rising paths, called jumps, as a result of a number of passing bubbles. Soria-Verdugo et al. [6] also characterized this behavior experimentally in a 2D bed for a neutrally-buoyant object. The buoyancy effects were also analyzed for several configurations, varying the operational conditions of the bed (gas velocity and bed aspect ratio) and the object properties (density and aspect ratio) obtaining no differences for these probabilities for objects with a proper circulation throughout the bed [7]. They proved that an object had a probability of 45% of reaching directly the surface of the bed and thus, a complementary probability of 55% of detaching from the bubble. Pallarès and Johnsson [8] observed the influence of bubble paths in the lateral motion of objects using a tracking technique in a 2D fluidized bed. They showed that two solid mixing vortices are produced around each preferential bubble path at the middle of the vortices. In the case of 3D beds, toroidal structures can be found around the bubble preferential path, [10]. These bubble paths are

affected by the operational conditions, the pressure drop of the distributor and the characteristics of the bed material. In a narrow 2D bed just one bubble path is observed at the center of the bed ([6] and [8]), while for wider beds other bubble paths appear and the configuration with two mixing vortices around the bubble path is repeated, in what is called a mixing cell, [9]. The interchange of particles between different vortices generates a net particle lateral motion. This structure of mixing cells and the lateral mixing of fuel particles in a large scale 3D fluidized bed was studied by [10].

The mixing rate in the vertical direction in fluidized beds is higher than that in the lateral direction due to the action of bubbles, [11]; nevertheless the latter is relevant in some applications. The lateral motion and the thermal conversion of a fuel particle are key parameters in the performance of a fluidized bed reactor. The relation between both parameters is represented by the Damkholer number (Da) defined, for horizontal processes, as the ratio of the lateral transport time and the thermal conversion time of a fuel particle, [12]. For high Damkholer numbers ($Da \gg 1$) the conversion process dominates and the thermal conversion of the fuel particle occurs close to the feeding port. On the other hand, for low Damkholer numbers ($Da \ll 1$) the lateral motion is faster than the thermal conversion process, producing a better distribution of fuel particles throughout the bed. The lateral motion of an object can be described by the lateral dispersion coefficient. Several authors have determined experimentally the lateral dispersion coefficient in both 2D and 3D fluidized beds using different techniques, and obtaining values in a range between $3 \cdot 10^{-4}$ and $0.14 \text{ m}^2/\text{s}$, as reviewed by [10]. For 2D beds, Salam et al. [13] and Xiao et al. [14] employed solids concentration sampling to obtain the lateral dispersion coefficient, whereas Pallarès and Johnsson [8] used a tracking technique of fuel particles. In 3D beds, defluidized bed sieving and residence time distribution were employed by [15] and [16] respectively. Olsson et al. [10] obtained the lateral dispersion

coefficient experimentally in a large-scale 3D fluidized bed using a tracking technique for different gas velocities. On the other hand, the thermal conversion processes during the lateral motion of the fuel particle in the bed can be characterized, distinguishing two main reactions: devolatilization and char combustion, [17]. The lower reaction time corresponds to devolatilization processes. The devolatilization time has been measured in the literature as a function of the fuel particle size and shape, obtaining values between 20 and 350 s, [18] - [20].

In this work, a Monte Carlo global model capable of describing the overall motion of a fuel particle with a proper circulation in a 3D large-scale fluidized bed is proposed. The model consisted of a combination of two Monte Carlo sub-models for the fuel particle motion inside the dense bed and in the freeboard. The motion of a fuel particle in the freeboard was described experimentally as a ballistic motion in a 2D fluidized bed by [21], obtaining the lateral displacement and the time of flight of the fuel particle in the freeboard. For the fuel particle motion inside the bed, the circulation time of a fuel particle during a cycle, from the bed surface to a certain depth and back to the surface, was analyzed experimentally for different operational conditions and fuel particles characteristics in a 3D lab-scale fluidized bed by [22]. This circulation time was also modeled by [23] using Monte Carlo simulations and obtaining good agreement with experimental results for 2D and 3D lab-scale fluidized beds. The lateral displacement of a fuel particle inside the bed and the extension of the two sub-motion models to a large-scale 3D fluidized bed were considered in a Monte Carlo global model in this work. The results obtained in the Monte Carlo global model were compared with experimental data for the lateral dispersion of fuel particles reported by [10], obtaining a good agreement. The influence of the bed operational conditions on the lateral mixing was also analyzed, obtaining the maximum lateral displacement of the fuel particle for different residence times. Comparing these residence

times with the fuel devolatilization time, an optimal distance between feeding ports was determined for a proper distribution of the fuel through the bed.

2. Theoretical Model

A model based on Monte Carlo simulations is proposed to characterize the overall motion of a fuel particle with a proper circulation in a 3D fluidized bed operated at ambient conditions. The global motion can be divided in two sub-motions; i) a motion of the fuel particle immersed in the bed and ii) a motion of the fuel particle in the freeboard. The different behaviors were studied in separated sub-models and combined to generate a global model.

2.1. Vertical motion of a fuel particle inside the bed

The fuel particle vertical motion when it is immersed in the bed was described based on a 1D Monte Carlo simulation, [23]. The total height of the bed was divided in $n=10$ slices with a length of 0.04 m, associating each one, j , with a different depth. The number of slices was selected to be high enough to properly describe the vertical path of the fuel particle in the bed and to count on a length higher than the fuel particle size. The initial position of the fuel particle at the surface of the bed corresponded to a depth equal to zero, $j=0$. The maximum depth attained was the total height of the bed, when the fuel particle reached the bottom of the bed, $j=n$. The fuel particle motion inside the bed started at the bed surface. Then, the fuel particle sank in the bed and circulated through it and finally came back to the surface in what is called a cycle. In a cycle, the fuel particle can move downwards with the dense phase material in a sinking process or upwards due to the effect of passing bubbles in a rising process. There could be several rising paths in a cycle, with a rising motion composed of several jumps, as previously reported in the literature by [5], [6].

The model was based on three external parameters: the probability of a fuel particle to start a rising path when it is in a sinking process, q , the probability of a fuel particle to move directly to the bed surface when it starts a rising path, p , and a parameter that establishes the position, i , where the fuel particle detached from the bubble, ending its rising path prior to arriving to the bed surface. The probability of a fuel particle to start a rising path, q , varies with the depth according to the motion of a fuel particle with a proper circulation throughout the bed, [23]. In Eq. 1 the probability density function of q is presented for a bed of 0.4 m in height.

$$q(d) = 1.667 \cdot e^{-0.8585d} + 0.0042 \cdot e^{18.93d} \quad \text{Eq. 1}$$

where d represents the depth of the fuel particle in the sinking path.

The probability of a fuel particle to reach directly the surface, p , was studied experimentally by [7]. The results showed a constant value of p equal to 0.45 in the whole bed for several bed conditions (aspect ratio and dimensionless gas velocities) and fuel particle properties (aspect ratio and density). Therefore, when a fuel particle starts a rising path at any depth, there is a probability of 45%, $p=0.45$, to get the surface directly and a complementary probability, $1-p=0.55$, to detach from the bubble. The last external parameter in the vertical motion model inside the bed is the depth, i , where the fuel particle is detached from the rising path when the surface is not reached directly. The effect of this parameter was analyzed in [23], concluding that the assumption that the fuel particle detached from the bubble in the position immediately before, $j-1$, of that where the rising path started, j , provided a good agreement with experimental results. The location where the fuel detaches from the bubble may have an effect on the vertical path followed by the fuel particle; nevertheless the effect on the circulation time, which is the important parameter for the determination of the lateral fuel dispersion, is negligible.

The Monte Carlo simulation of this motion followed the procedure schematized in Fig. 1. A fuel particle begins at the bed surface, $j=0$, and starts the sinking process arriving to the next depth, $j=1$. There, a random number, N_q , following a uniform distribution between 0 and 1 is generated. If the number is higher than the probability to start a rising path in this position $q(d(j))$, the fuel particle continues sinking to the next position, $j+1$, and another uniformly distributed random number N_q is generated. Otherwise, the fuel particle starts a rising path, and another uniformly distributed random number, N_p , is generated. If this number is higher than the probability of reaching the surface directly, $p=0.45$, the fuel particle is detached from the rising path and falls in the previous position, $j-1$, and the sinking path continues to the following slice where a new bubble could raise the fuel again. On the other hand, if the number, N_p , is lower than 0.45 or the position where the fuel particle detached is $j=0$, the fuel particle gets the surface directly and a new cycle starts.

[Figure 1 about here]

From the parameters described above, the vertical trajectory of a fuel particle for each cycle was obtained. Nevertheless, to obtain a time scale characterization, the sinking and rising velocities of the fuel particle were needed. The model can be employed to describe the motion of fuel particles with slight buoyancy effects, but still with a proper circulation throughout the bed, since the value of p was determined to be equal for these particles by [7] and the value of q might be assumed to be similar. The only difference caused by this slight buoyancy of the fuel particles will be in the fuel particle sinking velocity. The sinking velocity for a neutrally-buoyant fuel particle was considered equal to that of the dense phase downwards velocity, v_{dp} , [3], [6] and can be calculated employing the Kunii and Levenspiel [24] correlation (Eq. 2). The fuel particle velocity in the rising path can be related with 20% of the mean bubble velocity [4], [6]. The bubble diameter in a 3D fluidized bed, D_B , was calculated using the Darton [25] equation (Eq. 3), and the bubble velocity,

U_B , was obtained using the Davidson and Harrison [26] correlation (Eq. 4). Both the sinking and rising velocities of a particle with slight buoyancy effects can be found in [7]. The values of the velocity employed in the results presented in this work are those of a neutrally-buoyant particle for simplicity, nevertheless the effect of buoyancy forces on the fuel particle velocity is slight.

$$v_{dp} = \frac{f_w \delta U_B}{1 - \delta - f_w \delta} \text{ Eq. 2}$$

$$D_B = \left[0.54 (U - U_{mf})^{0.4} (h + 4\sqrt{A_0})^{0.8} \right] / g^{0.2} \text{ Eq. 3}$$

$$U_B = U - U_{mf} + \phi \sqrt{g D_B} \text{ Eq. 4}$$

Where the downwards velocity of the dense phase, v_{dp} , depends on the bubble wake fraction, f_w , the bubble fraction in the bed, δ , and the bubble velocity, U_B . The bubble diameter, D_B , is a function of the gas velocity, U , the minimum fluidization velocity, U_{mf} , the height over the distributor, h , and the area of the distributor per number of orifices A_0 . Finally, ϕ is a constant determined experimentally.

Once the velocity of the fuel particle and its vertical trajectory were determined, the circulation time, needed for the fuel particle to complete a cycle inside the bed, was calculated. Furthermore, the maximum depth reached by the fuel particle in each cycle was also calculated. Thus, the outputs of the model inside the bed are the circulation time and the maximum depth reached by the fuel particle in each of the N cycles. The procedure and the results of the Monte Carlo simulations were validated experimentally with data from 2D and 3D fluidized beds in a previous work [23] showing a good agreement.

2.2. Freeboard motion

The motion of a fuel particle in the freeboard of the bed was characterized by [21] for different bed conditions (dimensionless gas velocities and fixed bed heights). The fuel particle motion was a ballistic motion, only affected by gravity (being the drag force negligible), and defined by the ejection velocity of the fuel particle characterized by the modulus and the ejection angle (angle between the velocity direction and the vertical axis). The experimental results obtained by [21] in a 2D bed showed a probability function for the ejection angle expressed by the exponential distribution of Eq. 5. The modulus of the mean ejection velocity of the fuel particle was found to be related to the mean bubble velocity and the cosine of the ejection angle (Eq. 6). The dimensionless ratio of the modulus of the ejection velocity to the bubble velocity times the cosine of the ejection angle showed a Gaussian distribution with a mean of 1.00 and standard deviation of 0.32.

$$p_{ang}(\theta) = 0.046 \cdot e^{-0.045\theta} \text{ Eq. 5}$$

$$\overline{U}_{fp} = U_B \cos \theta \text{ Eq. 6}$$

where p_{ang} is the probability function of the ejection angle, θ is the ejection angle and \overline{U}_{fp} is the modulus of the mean ejection velocity of the fuel particle.

Once the modulus of the ejection velocity and the ejection angle were obtained, the time spent by a fuel particle following its ballistic motion, time of flight, t_f , and the lateral displacement in the freeboard, Δr , can be calculated using the ballistic equations. The time of flight and the lateral displacement in the freeboard were calculated as a function of the modulus of the ejection velocity and the ejection angle of the fuel particle by Eq. 7 and Eq. 8 respectively.

$$t_f = \frac{2 \cdot U_{fp} \cos \theta}{g} \text{ Eq. 7}$$

$$\Delta r = U_{fp} \sin \theta \cdot t_f \text{ Eq. 8}$$

where t_f represents the time of flight, Δr , the lateral displacement in the freeboard and U_{fp} the modulus of the ejection velocity of the fuel particle.

A Monte Carlo model was proposed to obtain the time of flight and the lateral displacement of a fuel particle for N cycles. The inputs of the simulation were the density function of the ejection angle and the Gaussian distribution of the relation between the modulus of the ejection velocity of the fuel particle and the bubble velocity characterized by Eq. 5 and Eq. 6 respectively. The outputs of the simulations are N values of time of flight and lateral displacement of the fuel particle in the freeboard.

2.3. Global motion

The Monte Carlo models for the fuel particle motion inside the dense bed and in the freeboard were combined to describe the global motion of a fuel particle in a large-scale 3D fluidized bed. The 3D bed dimensions and the mixing cells distribution were chosen similar to that reported by [10], considering a typical fuel particle size around 2 cm. They presented several experimental data for the lateral dispersion of a fuel particle which were used to validate the proposed model in this work. The lateral motion of the fuel particle inside the bed was calculated based on the mixing cells distribution.

The initial position of a fuel particle is at the surface of the bed. The fuel particle is submerged inside the bed, and this motion is characterized by the sub-model of the fuel particle motion inside the bed described in section 2.1. Therefore, the circulation time and the maximum depth reached by the fuel particle in a cycle were obtained. The lateral

displacement of the fuel particle inside the bed was determined depending on the maximum depth reached by the fuel particle. If the maximum depth is small, the fuel particle would describe a short cycle inside the bed and the position where it reappears at the surface will be near to the position where it sank. On the other hand, if the fuel particle describes a large cycle inside the bed, i.e. higher depths reached, it can reappear farther from the sinking point in the same mixing cell or even in a neighboring mixing cell.

When the fuel particle describes a short cycle with a maximum depth, d_m , lower than the mean bubble diameter at the top of the bed, D_B , the lateral displacement must be low. Therefore, the emersion point should be close to the sinking point, being the maximum lateral displacement inside the bed similar to the bubble diameter. Thus, the fuel particle emersion position was calculated using a Gaussian distribution, centered at the sinking point of the fuel particle, and assuming that the mean bubble diameter was three times the standard deviation. This case is schematized in Fig. 2a, where the fuel sinking point in a bed with four mixing cells is plotted. The dense phase circulation is depicted in black and the probable path of the fuel in blue. At the bed surface, the probability density function of the emersion point at each position is also given.

On the other hand, when the cycle described by the fuel particle is large, i.e. the maximum depth, d_m , reached is higher than the mean bubble diameter at the top of the bed, D_B , the lateral displacement inside the bed can be higher. In this case, the cycle is more probably composed of several jumps, and the fuel particle might reappear at the surface in the same mixing cell than the sinking point or in a neighboring mixing cell. The probability of a fuel particle to appear in a mixing cell is inversely proportional to the distance between the center of each mixing cell and the fuel particle sinking point. Since the preferential path in a mixing cell is located at the center [8], the fuel particle emersion point was calculated as a Gaussian distribution centered at the center of the corresponding mixing cell, with half

the lower size of the mixing cell as three times the standard deviation. A schematic of this process is given in Fig. 2b, where it can be observed that the emersion point can be found at the same mixing cell than the sinking point or even in a neighboring cell.

[Figure 2 about here]

Both for short and large cycles, the azimuth angle was assumed to be equiprobable. Therefore, the position of the fuel particle when appearing at the surface is determined and the lateral displacement inside the bed can be calculated. The lateral displacement inside the bed is considered as the distance from the fuel particle sinking point to the fuel particle emersion position.

The global motion of the fuel particle in the 3D bed was completed employing the model of the fuel particle motion in the freeboard. The lateral displacement in the freeboard and the time of flight were obtained and the position where the fuel particle sank was calculated with an equiprobable azimuth angle. Therefore, the global motion of the fuel particle was completely characterized. The outputs of the global model are the positions where the fuel particle emerged and sank at the bed surface, the circulation time inside the bed and the time of flight in the freeboard. Thus, the displacement in a global cycle, both inside the bed and in the freeboard, was calculated as the distance between consecutive sinking points and the global cycle time as the sum of the circulation time and the time of flight. Finally, a number of global cycles, N , with their respective displacements and times were obtained for all the fuel particles simulated, N_{fp} .

3. Results and discussions

3.1. Validation of the model with experimental results from the literature

The Monte Carlo global model proposed is valid fuel particles with a proper circulation throughout the whole bed and when they are only affected in the freeboard by gravitational forces. The assumptions of the sub-models and their results have been validated experimentally, as previously stated. Nevertheless, the assumptions for the lateral displacement inside the bed and the global motion presented in section 3.3 were not previously validated. Therefore, in this section the results of the Monte Carlo global model were compared with the results obtained experimentally in a large-scale 3D bubbling fluidized bed by [10]. The authors studied the lateral mixing of fuel particles in a commercial gasifier. The tests were performed at ambient conditions in a bubbling fluidized bed with a cross sectional area of 1.44 m², with rectangular shape, in the Chalmers indirect gasifier. The bed material was silica sand with a density of 2 600 kg/m³ and an average particle size of 150 μm. The fixed bed height was 0.4 m and the minimum fluidization velocity was 0.02 m/s. Two dimensionless gas velocities, U/U_{mf} , were employed by the authors in the experiments, 5 and 7.5. During the tests, two types of fuel particles, wood chips with a density of 523.5 kg/m³ and bark pellets with a density of 1178.6 kg/m³, were tracked. The fuel particles were covered with a phosphorescent plastic and recorded from above the bed surface using a CCTV camera at an acquisition frequency of 25 frames per second. The tracer particles were fed through a sampling port as a single particle or as a batch, formed by 14-20 particles. Therefore, the position of the fuel particles in the plane XY over the bed surface was obtained directly from the image.

Comparison of the lateral dispersion coefficient

The lateral dispersion coefficient is a useful parameter to analyze the lateral mixing of fuel particles in a large fluidized bed. Olsson et al. [10] calculated the lateral dispersion coefficient employing the Einstein equation [27], presented in Eq. 9. The mean lateral dispersion coefficient was determined for the batch experiments by averaging the

individual values over a time interval between 1 and 7 min. In case the fuel particle hit the walls at any moment before 7 min, just the values up to that instant were considered in order to avoid wall effects.

$$D_k = \frac{\sum_{i=1}^M (\gamma_k^2 / 2\Delta t)_i}{M} \quad k = x, y \quad \text{Eq. 9}$$

where D is the lateral dispersion coefficient, γ the lateral displacement and Δt is the cycle time.

In order to compare the results reported by [10] for the lateral dispersion coefficient with the results of the Monte Carlo global model, a series of simulations were carried out following the characteristics of the experimental facility. The geometry and the characteristics of the bed and the mixing cells in the simulations were equal to the experiments. The height of the bed was divided in ten slices of 0.04 m in order to characterize the vertical behavior of the fuel particle inside the bed. The time simulated was the same than that used in the experimental results, a time interval between 1 to 7 min corresponding to an average number of cycles, N , of 34. The wall effect was also considered stopping the simulation if the fuel particle hits the wall. For each cycle, the lateral dispersion coefficient was calculated according to Eq. 9 for x and y-direction, and the average in the N cycles was obtained for a fuel particle. Finally, 10 000 fuel particles were simulated in order to obtain a representative statistical data for the lateral dispersion coefficient. The results obtained by the Monte Carlo global model are plotted in Fig. 3 in the form of a box plot for different gas velocities, together with the experimental results of [10]. The median value, the upper and lower quartile, corresponding with 75% and 25% of the population, and a confidence interval are given in the box plots. No outliers are depicted in order to clarify the figure.

[Figure 3 about here]

Fig. 3 shows a good agreement between the experimental data of [10] and the results of the Monte Carlo global model. The lateral dispersion coefficient increases with the gas velocity, since larger bubbles are produced and therefore the fluidization is more vigorous, concluding in a greater motion of the fuel particles. A small degree of anisotropy between the x-direction and y-direction was observed, being the dispersion coefficient in the y-direction higher than the x-direction because of the rectangular shape of mixing cells.

Comparison of the time and lateral displacement inside the bed

The ratio of the circulation time and the lateral displacement of a fuel particle inside the bed to the global time and global lateral displacement (both, inside the bed and in the freeboard) were calculated for the Monte Carlo global model and compared with the experimental results reported by [10] for a wood chip particle. The results of the simulations were calculated for a time interval of 7 min, according to the experimental procedure. The total circulation time of a fuel particle inside the bed was calculated as the sum of all the circulation times inside the bed for each cycle, whereas the global time was considered as the sum of the circulation times inside the bed and the times of flight in the freeboard during 7 min. For the lateral displacement, the ratio of the lateral displacement inside the bed to the global lateral displacement was calculated in a similar way to the time. In order to obtain a representative statistical result, 10 000 fuel particles were simulated. The comparison between the results of the Monte Carlo global model and the experimental results is shown in Table 1 for two different dimensionless gas velocities.

[Table 1 about here]

The results of the Monte Carlo global model show a good agreement with the experimental data of [10] for the $U/U_{mf} = 7.5$ case. More discrepancies were observed in the case of

$U/U_{mf} = 5$, which can be attributed to buoyancy effects in the wood chip particle during the experimental tests. The low ratio between the density of the wood chip and the bed material density involved a flotsam behavior. For low dimensionless gas velocities, the buoyancy effects made the fuel particles float at the surface of the bed, increasing the time spent by the particles at the bed surface and thus decreasing the ratio t_{inside}/t_{tot} . On the other hand, when the dimensionless gas velocity is increased to $U/U_{mf} = 7.5$ a more vigorous fluidization is produced, diminishing the buoyancy effects and preventing the fuel particle to float at the surface of the bed, increasing the ratio t_{inside}/t_{tot} . This reduction of buoyancy effect when the dimensionless gas velocity increases, has been previously reported by [28], [7]. The model proposed in this work considers fuel particles with a proper circulation throughout the bed and velocities similar to that of a neutrally-buoyant particle and thus, the discrepancies were more important for the case of $U/U_{mf} = 5$ when buoyancy effects on the fuel velocity are significant and a poor circulation of the fuel in the bed is obtained. From the results of this section it can be concluded that the results of the Monte Carlo global model and the experimental results reported by [10] showed a good agreement provided that the fuel has a proper circulation in the bed. Therefore, the Monte Carlo global model proposed describes accurately the fuel particle behavior in a 3D fluidized bed.

3.2. Determination of the cumulative probability distribution

Once the Monte Carlo global model was validated with experimental data, several results were obtained from the simulations. The geometry of the bed and mixing cells employed for these results are still those of the experimental facility described by [10]. The presence of the fuel particle at the surface of the bed was characterized by the cumulative probability distribution of observations. The number of times that the particles were detected at the surface of each mixing cell was obtained from the Monte Carlo simulations

over a time interval of 7 min employing an acquisition frequency of 25 frames per second. Therefore, the position of a fuel particle at this discretized times was determined during 7 min and the number of times that the fuel particle was found at the surface of each mixing cell was calculated. In order to obtain a proper statistics, 10 000 fuel particles were simulated. The cumulative probability distribution of observations per unit of mixing cell area obtained from the Monte Carlo global model is plotted in Fig. 4 for two dimensionless gas velocities: 5 and 7.5. The initial position of the fuel particle in the simulations is marked with a filled circle according to [10].

[Figure 4 about here]

The presence of the fuel particle in the surroundings of the feeding port is higher than at farther distances, which are practically unavailable for the fuel particles in 7 min for both dimensionless gas velocities. Nevertheless, for the lowest dimensionless gas velocity, the fuel particle remains closer to the feeding port than for the higher dimensionless gas velocity. This occurs because of the lower lateral dispersion coefficient for $U/Umf = 5$ than for $U/Umf = 7.5$, which prevents the fuel particle to distance from the feeding port. The decrement of the values in the x-direction is smoother than in the y-direction due to the rectangular shape of the bed and the mixing cells. The results obtained by the Monte Carlo global model were found to be similar to the results of the model reported by [10].

3.3. Determination of the lateral dispersion coefficient for different gas velocities

In this section, new simulations were performed in order to study the influence of the bed walls on the lateral dispersion coefficient values, and its variation with the dimensionless gas velocity. The convergence of the results as a function of the time considered for the simulations was also analyzed.

Fig. 5 shows the variation of the mean value of the lateral dispersion coefficient with the number of global cycles for a fuel particle simulated with the Monte Carlo global model, for a dimensionless gas velocity of 5. The lateral dispersion coefficient in the x-direction, D_x , the y-direction, D_y , and the radial direction, D_r , were calculated considering no bed limits.

[Figure 5 about here]

The lateral dispersion coefficient shows scattering for a low number of global cycles, nevertheless a constant value was reached for a high number of cycles. The number of cycles needed in the simulations to obtain a constant value of lateral dispersion coefficient was above 10 000 global cycles, as can be observed in Fig. 5. This number of global cycles is much higher than that employed in the simulations for the experimental comparison, just 34 cycles, obtaining in that case a higher dispersion in the values (see Fig. 3). In order to study the effect of the number of cycles, i.e. the time considered, on the scattering of the lateral dispersion coefficient 100 000 fuel particles were analyzed.

The limits of the scattering of the lateral dispersion coefficient in the radial direction are shown in Fig. 6 as a function of the number of global cycles for a dimensionless gas velocity of 5. The limits represent the fitting of the maximum and minimum values of the lateral dispersion coefficient obtained for 100 000 fuel particles simulated, with an average cycle time equal to 13 s. The scattering found in the literature for the lateral dispersion coefficient might be attributed to the effect of the time considered in the calculation or in the measurement. As can be observed in Fig. 6, the lateral dispersion coefficient varied between 10^{-8} and 10^{-2} m²/s for low times in the case of a dimensionless gas velocity of 5. The range of variation diminished when increasing the time considered. Nevertheless, the mean value of the lateral dispersion coefficient is uniform with the number of cycles considered, when analyzing 100 000 fuel particles.

[Figure 6 about here]

The influence of the dimensionless gas velocity in the lateral dispersion coefficient in the radial direction has also been analyzed in the simulations. The value of U/U_{mf} was varied from 2 to 8 for the general configuration without bed limits. The statistical distribution of the lateral dispersion coefficient is presented in Fig. 7a in the form of a box plot for just one fuel particle with 100 000 global cycles at different U/U_{mf} . No outlier is depicted in the figure for clarifying purposes. The mean value of the distribution is also plotted in Fig. 7a marked with a cross. Fig. 7b shows the mean and median values of the lateral dispersion coefficient and the parabolic fitting for both values, as a function of the dimensionless gas velocities.

[Figure 7 about here]

An increment in the dimensionless gas velocity involves a higher lateral dispersion coefficient as can be observed in Fig. 7a. The scattering of the lateral dispersion coefficient also increases with the dimensionless gas velocity. The increase of the lateral dispersion coefficient of a fuel particle with the gas velocity is in accordance with the results already reported in the literature by several authors, [8], [9], [13]. The increase of the mean and median values of the lateral dispersion coefficient with the dimensionless gas velocity is parabolic, as can be seen in Fig. 7b. A determination coefficient R^2 of 0.997 and 0.994 was obtained for the parabolic fitting of the mean and median values respectively. The maximum discrepancies of the mean and median values of the lateral dispersion coefficient for 100 fuel particles is lower than 1.6% and 2.3% respectively for all the dimensionless gas velocities.

The distributions of the lateral dispersion coefficient for the x and y-directions were also obtained for dimensionless gas velocities U/U_{mf} between 2 and 8, the results are plotted in

Fig. 8. The lateral dispersion coefficient for both directions increases with the dimensionless gas velocity, following again a parabolic distribution for the mean and median values.

[Figure 8 about here]

3.4. Characterization of the feeding port distance for different configurations

The location of the feeding ports in a fluidized bed combustor is a key parameter in order to obtain a homogenous thermal conversion of the fuel particle in the bed, avoiding the formation of hot or cold spots. The optimal location and number of the feeding ports are defined when the fuel particles can be distributed homogeneously to the whole bed. An optimal distribution of the feeding ports would produce higher thermal conversion efficiencies and a reduction of the maintenance costs.

The residence time of the fuel particle in the bed is another key parameter in the performance of fluidized bed reactors and thus it should be considered in the feeding port location determination. This residence time can be associated to the time during a devolatilization process of a fuel particle. The motion of the fuel particle in the bed during the devolatilization process involves different mixing behaviors described by the Damkohler number as stated in the section 1. Several authors have determined experimentally the devolatilization times of biomass fuel particles as a function of size and shape. De Diego et al. [18] and Wang et al. [19] obtained devolatilization times between 20 and 250 s for wood fuels at different temperatures, while for Srekanth et al. [20] the values range between 50 and 350 s also for wood particles.

In this work, simulations were performed to study the maximum lateral displacement for different number of global cycles and dimensionless gas velocities. The global time employed in each simulation varied from 30 to 360 s in intervals of 30 s, according to the

devolatilization times reported in the literature. The different dimensionless gas velocities, U/U_{mf} , used were 2, 4, 6 and 8. Four different configurations were considered in the simulations, three of them using the bed geometry reported by [10], varying the initial position of the fuel particle in the simulations, as showed in Fig. 9, and one more without bed limits, just for comparison with the results considering the bed geometry.

[Figure 9 about here]

The total number of fuel particles simulated was 10 000 for each configuration, devolatilization time and dimensionless gas velocity. The distance between the farther position reached by the fuel particle and the injection point was calculated for different devolatilization times and gas velocities. The optimal distance between feeding ports were estimated as two times the median value of the largest distance calculated for the 10 000 fuel particle. In Fig. 10, the optimal feeding port distance is plotted as a function of the devolatilization time, for all the dimensionless gas velocities and configurations.

[Figure 10 about here]

The optimal distance between feeding ports increases with the dimensionless gas velocity and the devolatilization time for all configurations because of the larger lateral displacement of the fuel particle. This increment of the optimal feeding port distance depends on the position of the feeding port. For the dimensions of the bed simulated, where the distance between the horizontal walls (y-direction) was lower than between the vertical walls (x-direction), the results vary. For devolatilization times up to 90 s, the variation of the optimal feeding port distance is similar for all the configurations. After that instant, for the vertical and interior configurations, the increment of the optimal feeding port distance with U/U_{mf} is smoother than in the case of the horizontal initial position or the case without walls. This smoother increment shall be attributed to the hits of the fuel

particle with the horizontal bed limits in the vertical and interior configurations, whereas the bed limits are farther to the initial position for the horizontal configuration. In the results of the configuration without bed limits no changes in the variation of the optimal feeding port distance are observed for the range of devolatilization times simulated, as can be seen in Fig. 10d. The optimal distance between feeding ports for the horizontal configuration is quite similar to the case without walls, showing differences just for high devolatilization times and gas velocities when the lateral displacement of the fuel particle is comparable to the distance to the walls. Finally, the results of the optimal feeding port distance reported in Fig. 10 could be employed to determine the optimal number of feeding ports for a particular bed geometry.

4. Conclusions

A model based on a Monte Carlo method was developed to describe the motion of a fuel particle with a proper circulation throughout the bed in a large scale 3D fluidized bed. The global motion was divided in two sub-motions, the motion when the fuel particle is immersed in the dense bed and the motion in the freeboard. The results obtained from the Monte Carlo global model were compared with experimental results reported in the literature, showing a general good agreement for fuel particles with a proper circulation in the bed. The lateral dispersion coefficient was calculated for several dimensionless gas velocities, between 2 and 8, showing an increment of the lateral dispersion coefficient with the dimensionless gas velocity. The time considered in the determination of the lateral dispersion coefficient affects the scattering obtained, being higher for lower times. This scattering is also larger for high dimensionless gas velocities.

The optimal distance between feeding ports was calculated for several configurations, varying the feeding port location, considering typical values for the devolatilization times of fuel particles. For higher dimensionless gas velocities and devolatilization times the

optimal distance between feeding ports was larger. Finally, for a particular bed geometry, the optimal number and location of feeding ports to guarantee a proper distribution of fuel particles throughout the bed can be calculated from the results presented in this work.

Nomenclature

A_0	Area of the distributor per number of orifices [m ²]
d	Depth inside the bed [m]
D	Lateral dispersion coefficient [m ² /s]
D_B	Bubble diameter [m]
D_r	Lateral dispersion coefficient in the radial direction [m ² /s]
D_x	Lateral dispersion coefficient in x-direction [m ² /s]
D_y	Lateral dispersion coefficient in y-direction [m ² /s]
f_w	Bubble wake fraction [-]
g	Gravity [m/s ²]
h	Height over the distributor [m]
L	Bed length [m]
L_{inside}/L_{tot}	Ratio of the lateral displacement inside the bed to the global lateral displacement of the fuel particle [-]
N	Number of cycles simulated [-]
N_q	Random number [-]
N_p	Random number [-]
p	Probability of a fuel particle to get to the surface [-]
p_{ang}	Probability function of the ejection angle [-]
q	Probability of a fuel particle to start a rising path [-]
t	Cycle time [s]
t_{dev}	Devolatilization time [s]
t_{inside}/t_{tot}	Ratio of the time inside the bed to the global time of the fuel particle [-]
t_f	Time of flight [s]

Δr	Lateral displacement in the freeboard [m]
U	Superficial gas velocity [m/s]
U_B	Bubble velocity [m/s]
U_{mf}	Minimum fluidization velocity [m/s]
\overline{U}_{fp}	Modulus of the mean ejection velocity of the fuel particle [m/s]
U_{fp}	Modulus of the ejection velocity of the fuel particle [m/s]
v_{dp}	Downwards velocity of the dense phase [m/s]
W	Bed width [m]
δ	Bubble fraction in the bed [-]
γ	Lateral displacement [m]
λ	Constant determined experimentally [-]
ϕ	Constant determined experimentally [-]
θ	Ejection angle [deg]

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