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An algorithm to simulate packing structure in cylindrical containers

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Abstract

The aim of this work is to propose an algorithm to simulate the packed bed structure of mono-sized spheres in cylindrical containers. The approach employed is called soft spheres algorithm, because it allows some degree of interpenetration between particles. The force balance accounts for gravity and contact force (to take into account the interpenetration), and neglects the friction force between particles. The algorithm provides detailed information about packing structure so it can be employed to evaluate local and global properties. The results fit better the experimental information than previous algorithms from the literature.

Keywords: Packed bed generation; Packing structure; Catalytic fixed bed; Mono-sized spheres

1. Introduction

Cylindrical packed beds are widely used in almost all chemical process industries. Examples of paramount importance are catalytic fixed bed reactors with either single or two phase flow. In such type of units catalytic particles can have sizes fairly different from fine powders, often reaching several millimeters. The model employed to simulate the reactor determines the degree of information required about packed bed structure. For the nowadays increasing use of the computational fluid dynamics technique (CFD) it is necessary to state the positions of all particles [1].

Many packing structure studies have been made during the last decades from different points of view. Destructive and non-destructive techniques have been used to obtain packing information of different types, but the main interest has been the evaluation of void fraction [2–4].

With the aim of obtaining a quantitative description of the packed bed structure, and particularly of the radial void fraction profile, alternative approaches were carried out [5]. To predict the overall void fraction or radial void fraction distribution, empirical expressions have been proposed [3]. Parameters involved in those expressions were obtained by fitting the experimental data.

Another approach is based on accounting for the radial particle center distribution [6]. Expressions describing such distribution provide a more detailed description of the packing structure, a feature that is essential for certain models of packed bed processes considering the discontinuous nature of the solid phase.

Indeed, packing properties arise as a consequence of the location of the particles in the bed [7]. Hence, it is clear that the knowledge of the location of the particles is the more basic and complete information about the packing structure. Overall bed void fraction, radial and axial void fraction profiles, particle center distribution and external surface area profiles can be readily evaluated from the location of particles. Therefore, another strategy to conduct the studies on packed bed structure is the development of computational tools to obtain the position of each particle in the bed.

There is a considerable literature background on unbounded 3D spatial arrangements of particles, especially spheres. Nonetheless, the information is somewhat scarce when dealing with the arrangement of particles constrained

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Nomenclature

a	aspect ratio (=$(2R_t/D_p)$)
C_k^m	elasticity parameter at the m-th iteration (=$(k^m U^m)$)
C_g^m	gravity parameter at the m-th iteration (=$(MgU^m D_p^{-1})$)
D_p	sphere diameter (m)
$\vec{F}_{i,Bw}$	force exerted by the container's bottom on the i-th sphere (N)
$\vec{F}_{ij,C}$	contact force exerted by the j-th sphere on the i-th sphere (N)
$\vec{F}_{i,Lw}$	force exerted by the lateral wall on the i-th sphere (N)
$\vec{F}_{i,n}$	net force acting on the i-th sphere (N)
g	acceleration of gravity (m s^{-2})
k	elasticity coefficient (N m^{-1})
L	packing height (m)
M	sphere mass (kg)
N_p	total number of particles in the packing
$\hat{r}_{ij}$	unit vector defined from the center of the i-th sphere to the center of the j-th sphere
R_t	cylindrical container radius (m)
U^m	step-length at the m-th iteration (m N^{-1})
$\vec{W}$	sphere weight (N)
x	dimensionless distance from the wall (=$(R_t - \rho)/D_p$)
$\vec{x}_i^m$	location of the i-th sphere at the m-th iteration (m)
z_i	axial coordinate of the i-th sphere measured from the bottom of the bed (m)
$\hat{z}$	axial unit vector (upwardly oriented)

Greek letters

δ_{ij}	overlapping between i-th sphere and j-th sphere $= D_p - \|\|\vec{r}_i - \vec{r}_j\|\|_2$ (m)
δ_{iw}	overlapping between i-th sphere and the lateral wall, $= (\rho_i + D_p/2) - R_t$ (m)
$\delta_{ij,max}$	maximum value out of all δ_{ij} (m)
$\delta_{iw,max}$	maximum value out of all δ_{iw} (m)
ε_0	initial overall void fraction
ε_F	final overall void fraction
θ_i	azimuthal coordinate of the i-th sphere
ρ	radial coordinate measured from the container axis (m)
ρ_i	radial coordinate of the i-th sphere measured from the container axis (m)
$\hat{\rho}$	radial unit vector
$\|\|\cdot\|\|_2$	Euclidean norm

by cylindrical vessels. The distinctive attribute of these systems arises from the presence of the lateral walls and the floor that induce a highly ordered arrangement of particles nearby.

A primary classification of 3D algorithms to generate packed bed structure can be made by distinguishing between soft and hard sphere approaches, depending on the allowance of overlapping between spheres or not.

Pioneer works employing the soft sphere approach are those of Powell [8] and Jodrey and Tory [9] for simulating the structure of liquids. In such cases, the existence of the container wall is not taken into account. Hence, this kind of studies will not be considered later on when comparing different approaches.

Up to the best of our knowledge, all algorithms specifically described in the literature for confined packed beds, fall in the hard sphere category. Some of them will be commented on next, highlighting the different ways in which the dynamics of the generation of the packed bed is undertaken.

In the procedure known as random settlement [10–12], spheres are let down one at a time at random cross-section positions. When a sphere hits an already settled sphere no momentum transfer is considered, and the impinging sphere is allowed to slide down until a stable position is reached: on the base of the container, on three other spheres or on two other spheres and the cylinder wall. Schnitzlein [13] proposed a modified random settlement algorithm incorporating an optimization procedure for the packing.

Reyes and Iglesia [14] described structural properties of cylindrical packed beds employing a sequential random approach based on Monte Carlo method.

Mueller [15] analyzed four different deterministic algorithms: modified Bennett [16], layer, alternate and percentage methods. All procedures are initially assembled from a base layer at the bottom of the bed. Once the base layer is completed, there are two possible ways to allocate a new sphere: resting on three spheres from the lower layer (inner sites, IS) or resting on two spheres and the container wall (wall sites, WS).

It is worth noting that Mueller's calculations indicate that percentage model give the best results out of the options tried by the author. This method selects the lowest vertical location among all available WS or IS, depending on a given percentage. No update is made until all possible locations are filled. The procedure is repeated for additional layers until the desired number of spheres has been added.

The layer optimization method employed by Nandakumar et al. [17] relies on minimizing the bed height of a given number of non-overlapping particles. This number of particles is chosen to match a particle layer number. The minimization criteria arise from a mechanical analysis of the packing; without friction forces the system will arrange to minimize its potential energy, leading to the lowest mass center of the packing. The spheres belonging to the same layer do not move after the minimum height value was reached.

A relatively recent tool to model particulate systems is the Discrete Element Method (DEM) that has been widely used in many application fields [18]. However, up to the best of our knowledge, when dealing with the packing of

catalytic-type particles in cylindrical containers the DEM literature is scarce [19,20]. In addition, none of the mentioned articles deals with the wall effect, which is very important to evaluate transport processes in catalytic fixed beds and also, no systematic analysis of the aspect ratio influence, was carried out.

The basic and most widely used quantity to characterize packed bed structure is the overall bed void fraction. In this context, the algorithm predictions should be contrasted with experimental data for different aspect ratios. A good agreement turns out to be a necessary condition to guarantee a reliable tool.

Even when the results obtained with the previously described algorithms are encouraging, significant differences in macroscopic properties arise when contrasting with experimental information [5]. Hard sphere algorithms lead to loose packed bed, with overall void fraction values considerably greater than experimental ones.

The main goal of this contribution is to propose an algorithm to realistically simulate the structure of cylindrical packed beds with mono-sized spheres, as those employed as catalytic fixed bed. The algorithm is based on the soft sphere approach. The results obtained for the overall bed void fraction are compared with experimental information and with other simulations from literature.

2. Model formulation

For a packing of spheres in a cylindrical container an equilibrium condition is reached just when all forces acting on every particle are balanced. The forces acting on the particles are the gravitational field, friction and contact forces. Also, there are two physical restrictions to sphere accommodation: vessel and bottom walls.

It has been experimentally demonstrated that friction forces inhibit the compaction of the packing [21]. Besides, loose packing tend to become more compact by means of vibration [22] or after some period on operation. For these reasons, friction forces between particles and between particles and the vessel wall will not be considered, expecting that the algorithm formulation will provide results closer to real situations.

In order to model the effect of normal contact forces, a certain degree of interpenetration between the spheres will be allowed. The repulsion force generated from interpenetration is assumed to be proportional to the overlapping magnitude, as in elasticity theory. As described below, the intensity of this force will be effectively raised in the course of the procedure envisaged for the generation of the bed. In an early stage, the intensity of the repulsive force is kept relatively low, while in the final stage the intensity is increased so as to produce a very tiny overlap.

It will be shown that the effect gained from this strategy is the achievement of more compact beds, closer to those found in practice. At variance, previous models based on rigid spheres, as discussed in Section 1 of this paper, predict significantly looser beds.

The lateral wall of the container will also be considered as a deformable body. The force exerted by the lateral wall on a contacting sphere will point to the container axis.

The behavior of the base of the bed should also be defined. Although the base might be considered as being deformable too, it was checked that no definite effect is achieved through this assumption. Therefore, a rigid base exerting an action to balance the axial force on each resting particle on it will be assumed.

Summarizing, the following hypothesis are stated in formulating the algorithm to generate packed beds in cylindrical containers:

1. the spheres are mono-sized;
2. gravitational field is accounting for;
3. the friction forces are neglected;
4. the spheres as well as the lateral wall are deformable;
5. the base of the container is rigid;
6. the contact forces between spheres and between spheres and the wall are calculated relying on elasticity theory.

The net force $\vec{F}_{i,\mathrm{n}}$ acting on the i-th sphere can be expressed as:

$$\vec{F}_{i,\mathrm{n}} = \vec{F}_{i,\mathrm{Lw}} + \vec{F}_{i,\mathrm{Bw}} + \vec{W} + \sum_j \vec{F}_{ij,\mathrm{C}} \tag{1}$$

where $\vec{F}_{i,\mathrm{Lw}}$ is force exerted by the lateral wall on the i-th sphere; $\vec{W}$ is sphere weight; $\vec{F}_{ij,\mathrm{C}}$ is contact force exerted by the j-th sphere on the i-th sphere; $\vec{F}_{i,\mathrm{Bw}}$ is force exerted by the container's bottom on the i-th sphere.

All forces acting on every sphere pass through the center of the mass, therefore it is not necessary to set out the torque balances.

The formulation for every force is:

$$\vec{F}_{i,\mathrm{Lw}} = -kR(\delta_{i\mathrm{w}})\hat{\rho} \tag{2a}$$

$$\vec{F}_{ij,\mathrm{C}} = -kR(\delta_{ij})\hat{r}_{ij} \tag{2b}$$

$$\vec{W} = -Mg\hat{z} \tag{2c}$$

where $R(x)$ is Ramp function $= \begin{cases} 0, & \text{if } x \le 0 \\ x, & \text{if } x > 0 \end{cases}$; δ_{ij} is overlapping between i-th sphere and j-th sphere $= D_\mathrm{p} - ||\vec{r}_i - \vec{r}_j||_2$; $\delta_{i\mathrm{w}}$ is overlapping between i-th sphere and the lateral wall $=(\rho_i + D_\mathrm{p}/2) - R_\mathrm{t}$; $\hat{\rho}$ is radial unit vector; $\hat{z}$ is axial unit vector (upwardly oriented); $\hat{r}_{ij}$ is unit vector defined from the center of the i-th sphere to the center of the j-th sphere.

The forces $\vec{F}_{i,\mathrm{Bw}}$ are not formulated because it is supposed that their values are just enough to make zero the axial component of $\vec{F}_{i,\mathrm{n}}$ of those spheres contacting the bottom of the container.

It is worth remarking that $\vec{F}_{i,\mathrm{Lw}}$ and $\vec{F}_{ij,\mathrm{C}}$ are repulsive in nature and they become nil when there is no overlapping (Eqs. (2a) and (2b)). For the sake of simplicity the constant k is assumed to be the same for both, $\vec{F}_{i,\mathrm{Lw}}$ and $\vec{F}_{ij,\mathrm{C}}$.

Once the aspect ratio $a = 2R_t/D_p$ and the number of particles N_p are defined, the purpose of the algorithm described next is to define a set of positions for all particles that will render $\vec{F}_{i,n} = \vec{0}$ (in an approximate sense) for $i = 1, \ldots, N_p$.

3. Algorithm

The algorithm can be described considering four stages: generation, initial, intermediate and final stage. A set of images showing the packing structure in each stage of the simulation for $a = 5$, $N_p = 500$ and an initial overall void fraction $\varepsilon_0 = 0.47$ is depicted in Fig. 1.

The generation stage is needed to define an initial distribution of particles, while the other three stages are characterized by a specific effect on the packing structure (expansion, compaction, force balancing). Even when the division into stages is somewhat arbitrary, it arises as a result of tuning the algorithm to attain robustness and better convergence speed. The following quantities should be monitored to identify the transition between each stage: packing mass center (MC), maximum overlapping between particles ($\delta_{ij,max}$) and maximum overlapping between particles and the wall ($\delta_{iw,max}$).

Except in the generation stage, the reallocation of particles is guided by the need to reduce the net force ($\vec{F}_{i,n}$) acting on every sphere. From the values $\vec{x}_i^m$ and $\vec{F}_{i,n}^m$ at iteration m, the new location $\vec{x}_i^{m+1}$ of the i-th sphere is calculated as:

$$\vec{x}_i^{m+1} = \vec{x}_i^m + U^m \vec{F}_{i,n}^m \tag{3}$$

where U^m is the step-length chosen at iteration m. Substituting $\vec{F}_{i,n}$ according to Eqs. (2a) and (2b):

$$\vec{x}_i^{m+1} = \vec{x}_i^m - C_k^m \left[R(\delta_{iw}^m)\hat{\rho} + \sum_j R(\delta_{ij}^m)\hat{r}_{ij} \right] - C_g^m D_p \hat{z} \tag{4}$$

where

$$C_k^m = k^m U^m, \quad C_g^m = MgU^m D_p^{-1}, \tag{5}$$

are the elasticity and gravity parameters at iteration m. As the elasticity parameter will have to be changed in the course of the calculations, it is also written generically as dependent on the iteration level, k^m.

We can appreciate from definitions (5) that C_k^m and C_g^m can be employed to conduct the iterations, rather than the original parameters U^m and k^m. This has been the choice actually made. Both, C_k^m and C_g^m should be large enough to speed up the procedure towards the solution, but not too large to promote instabilities and final divergence. In addition, note that the ratio C_k^m/C_g^m should be made large towards the end of the calculations in order to relax the interpenetration between particles and between particles and the container wall.

It has been learned from numerical experience that keeping C_k^m fixed at $C_k = 0.3$, while varying C_g^m for the three stages described below (initial, intermediate and final), constitutes a simple and efficient approach. In the next section, the effect of changing the constant value C_k will be discussed.

3.1. Generation stage

To start the simulation, aspect ratio, a, and total number of spheres in the packing N_p are specified. The value of D_p is also assumed to be specified in the following description, although its magnitude will be irrelevant for the intrinsic properties of the generated bed.

An initial overall void fraction (ε_0) is assigned to evaluate the initial height of the bed:

$$L_0 = \frac{2}{3}\frac{D_p N_p}{a^2(1-\varepsilon_0)} \tag{6}$$

The N_p particles are then allocated, allowing overlapping between them, by assigning randomly the initial coordinates of their centers according to:

$$\begin{aligned} \rho_i &= \left(R_t - \frac{D_p}{2}\right)(\mathrm{Rnd})^{1/2} \\ \theta_i &= 2\pi\,\mathrm{Rnd} \qquad\qquad i = 1, \ldots, N_p \\ z_i &= L_0\,\mathrm{Rnd} + (D_p/2) \end{aligned}$$

where $\mathrm{Rnd} \in [0, 1]$ is a random number.

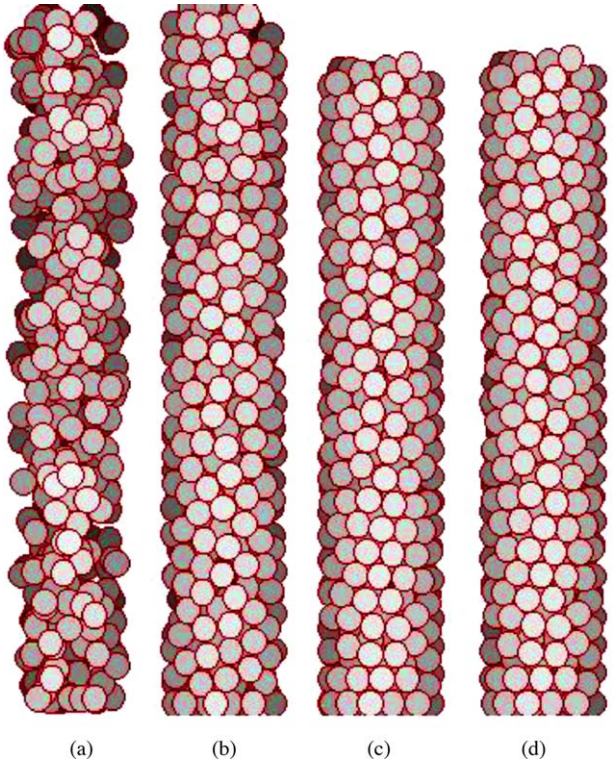

Fig. 1. Sequence showing the packed bed structure at the end of each simulation stage $a = 5$, $N_p = 500$, $\varepsilon_0 = 0.47$ and $\varepsilon_F = 0.433$. (a) Generation stage, (b) initial stage, (c) intermediate stage and (d) final stage.

3.2. Initial stage

The packing from the generation stage shows a significant number of overlapped spheres (see Fig. 1a). To lessen the degree of interpenetration, the gravity force on the spheres is suppressed, i.e. $C_g = 0$ is stated. Eq. (4) are then employed repeatedly until both, $\delta_{ij,\max}$ and $\delta_{iw,\max}$, become less than $1 \times 10^{-4} D_p$.

3.3. Intermediate stage

In the intermediate stage the packing is compacted under the gravity action. A control loop is implemented to adjust C_g^m for bounding the maximum overlapping between particles, $\delta_{ij,\max}$. An upper bound $\delta^U = 1 \times 10^{-2} D_p$ and a lower bound $\delta_L = 0.5 \times 10^{-2} D_p$ are established. Starting from a null initial value, C_g^m is varied according to:

$$C_g^{m+1} = \begin{cases} C_g^m + \Delta C_g, & \text{if} \quad \delta_{ij,\max} < \delta_L \\ C_g^m - \Delta C_g, & \text{if} \quad \delta_{ij,\max} > \delta^U \\ C_g^m, & \text{if} \quad \delta_L \le \delta_{ij,\max} \le \delta^U \end{cases} \tag{7}$$

The recommended step value of ΔC_g is 1.25×10^{-7}. A stationary value of C_g^m is eventually reached, typically around 2.0×10^{-5}. To end the intermediate stage, the packing mass center MC is evaluated after each set of 100 iterations. If 10 successive values of MC turn out to vary within 1×10^{-4}%, the intermediate stage is terminated.

3.4. Final stage

In the final stage, a slice modification of particle locations is carried out with the aim of reducing the overlapping up to the allowed value of $1 \times 10^{-4} D_p$. This stage is subdivided in several steps. For each step, C_g^m is maintained constant and its value is halved for the next step. Each step is terminated when the criterion on MC (as described above) is fulfilled. The whole stage is stopped when both, $\delta_{ij,\max}$ and $\delta_{iw,\max}$, become less than $1 \times 10^{-4} D_p$.

4. Sensitivity analysis of the algorithm's parameters

A set of simulations was carried out to analyse the effect of parameter assignment in the packing properties predicted by the foregoing algorithm. The studied quantities were: initial overall void fraction, ε_0, elasticity parameter C_k and the allowable range $[\delta_L, \delta^U]$ for $\delta_{ij,\max}$ in the intermediate stage (Eq. (7)). The same particle distribution from the generation stage was employed in all runs. The number of particles employed in the simulations was large enough to avoid end effects. The overall void fraction (ε_F) was selected to compare the generated packing structures.

4.1. Initial overall void fraction (ε_0)

The final packing was found to depend weekly on ε_0. For instance, at $a = 5$, if $\varepsilon_0 \in [0.30, 0.55]$, then $\varepsilon_F \in [0.43, 0.44]$. It is worth mentioning that the sensitivity increases as a decreases. For $a > 20$ there is no effect of ε_0 on ε_F.

4.2. Elasticity parameter (C_k)

By modifying the recommended value ($C_k = 0.3$) in 50%, the variation of ε_F was, on average, only 1%. Nonetheless, it is important to point out that modifying C_k strongly affects the time spent by the simulations. By raising the value of C_k the final solution, when reached, is obtained faster, but the chance for divergence increases. The suggested value ($C_k = 0.3$) arises from a trade off between the number of iterations and robustness.

4.3. Allowable range $[\delta_L, \delta^U]$ for $\delta_{ij,max}$ in the intermediate stage

The range $[\delta_L, \delta^U]$ employed to bound $\delta_{ij,\max}$ according to Eq. (7) was increased from the standard interval $[\delta_L, \delta^U] = [0.5, 1] \times 10^{-2} D_p$ up to $[\delta_L, \delta^U] = [14, 15] \times 10^{-2} D_p$. At $a = 5$, a reduction in ε_F from 0.431 to 0.427 was obtained. Larger values of aspect ratio were tried and it was checked that the effect on ε_F becomes less significant.

5. Overall void fraction estimation

The proposed algorithm provides the exact location of each particle in the bed. From this information, all the global and local properties of the bed can be estimated. As an example of the results that are currently being obtained [23], Figs. 2 and 3 show the comparison between Muller's experimental data [24] and the algorithm prediction for the radial particle center distribution and radial void fraction profile at $a = 7.99$. A remarkable agreement can be appreciated.

Aiming to carry out a systematic comparison among the proposed algorithm, other literature alternatives and experimental information, the overall bed void fraction was selected for two reasons. On one hand, any attempt to simulate a real packed bed structure should primarily provide a reliable prediction of ε_F. On the other hand, overall bed void fraction is largely the most intensively studied global property for a wide range of aspect ratios.

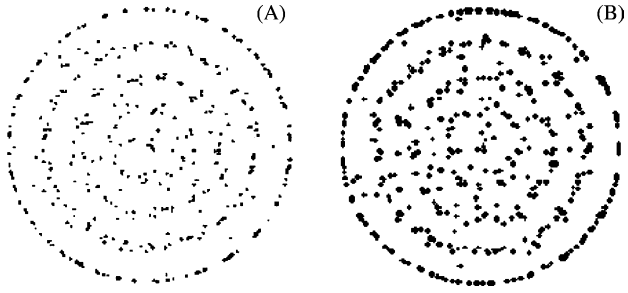

Fig. 2. Comparison between experimental and predicted radial particle centre distribution at $a = 7.99$. (A) Mueller [24]; (B) proposed model.

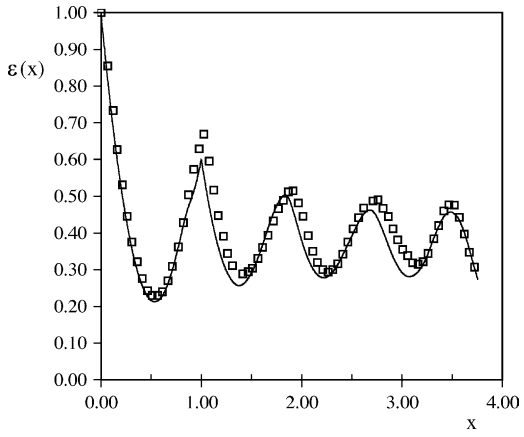

Fig. 3. Comparison between experimental and predicted radial void fraction profile at $a = 7.99$. (□) Mueller [24]; (—) proposed model.

An important number of simulations were carried out to cover a wide range of a, from 5 to 30, with the aim of testing the model performance.

In order to validate the results from the proposed model, experimental data and results from the proposed model can be compared in Fig. 4. Two empirical correlations [25] developed with the specific purpose of setting the boundaries for close and loose random packing in fixed beds were also added to Fig. 4. It can be concluded that the proposed algorithm can suitably represent the trend indicated by the experimental data. It closely reproduces most of the experimental data sets; particularly those placed within the boundaries stated from Zou and Yu [25] correlations.

Out of the whole set of available experimental data, the results from Fand and Thinakaran [26] and Limberg [27] provide the lowest values of ε_F. Note that they fall below Zou and Yu [25] random close packing correlation (Fig. 4). Additionally, for $a \to \infty$ (negligible container wall effects), Onoda and Liniger [28] concluded from the analysis of the experimental evidence that the minimum attainable value of ε_F is 0.363. Nonetheless, some of the values of Fand and Thinakaran [26] and Limberg [27] at large, but still finite values of a, are lower than Onoda and Liniger's limiting value.

The results from the proposed algorithm in Fig. 4 correspond to at least 10 runs for every a, each of them from a random generation stage. The interval markers show the spread of ε_F values. As previously pointed out by Mueller [15], randomness is an important feature to be included in algorithms for predicting packing structure because it avoids a strong bias in the generation stage.

A wider spread in the predicted values of ε_F as the aspect ratio diminishes is observed in Fig. 4. For lower aspect ratios, the different configurations that randomly arise for the packing structure nearby the vessel walls exert a stronger effect on the average value ε_F. On the contrary, for high aspect ratios (i.e. $a > 30$) random effects become negligible.

A comparison between results from the present algorithm and some literature algorithms is displayed in Fig. 5. Data from Reyes and Iglesia [14], Spedding and Spencer [12], Mueller's percentage model [15], Nandakumar et al. [17] and Schnitzlein [13] are included in Fig. 5. The upper correlation bound given by Zou and Yu [25] is also included in Fig. 5 as a reference set. It is clearly appreciated that most results from the literature models predicts higher values of ε_F than the reference upper bound. Thus, the mechanisms on which the literature algorithms are based introduce a strong bias, favoring much looser beds than supported by the experimental evidence. Besides, it is confirmed in Fig. 5 that the algorithm proposed here systematically produces more compact beds than previous alternatives.

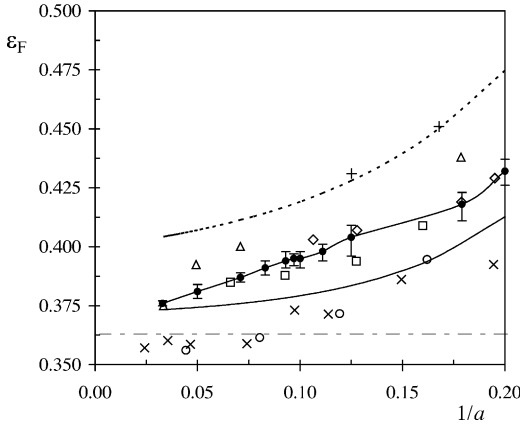

Fig. 4. Comparison between experimental and predicted overall void fractions (+) Mueller [3]; (△) Benenati and Brosilow [2]; (□) Carman [30]; (×) Fand and Thinakaran [26]; (◇) Dixon [29]; (○) Limberg [27]; (–●–) proposed model (different values resulting for each simulated aspect ratio are indicated by an interval); (—) Zou and Yu [25] random dense packing; (- - -) Zou and Yu [25] random loose packing; (– – –) Onoda and Liniger's [28] limiting value.

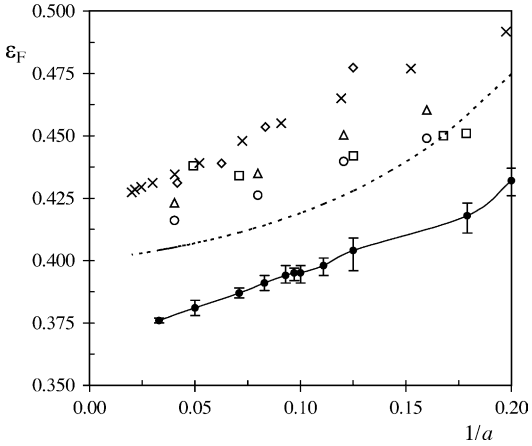

Fig. 5. Comparison between overall void fractions predicted by different simulations methods (×) Reyes and Iglesia [14]; (○) Spedding and Spencer [12]; (□) Mueller's percentage model [15]; (◇) Nandakumar et al. [17]; (△) Schnitzlein [13]; (–●–) proposed model (different values resulting for each simulated aspect ratio are indicated by an interval); (- - -) Zou and Yu [25] random loose packing.

6. Conclusions

An algorithm capable to describe the structure of cylindrical packed beds of mono-sized spheres has been presented in this work. It is based on stating a force balance on each sphere under certain assumptions. Friction force between the involved surfaces is neglected. Spheres particles and wall containers are considered as deformable bodies and, therefore a contact force arises. It is supposed that contact forces can be modeled from elasticity theory.

A particular feature of the algorithm is the randomness procedure proposed for the initial distribution of the particles. This feature intends to simulate the uncertainties associated with loading procedures of real packed beds.

The incidence of algorithm parameters on the predicted packing properties was assessed by comparing the final values of the overall void fractions, ε_F. Initial void fraction, relaxation parameter constant and bounds for the maximum allowed overlapping in the intermediate stage exert a mild effect on ε_F.

The quality of the results from the algorithm has been discussed in terms of the predicted values of ε_F. These values are satisfactorily consistent with the experimental data for a wide range of aspect ratio, taking into account the spread shown by the results from different sources.

It is also shown that the proposed algorithm performs definitely better than previous alternatives, due to the fact that more compact beds are predicted.

The algorithm provides a detailed information about packed bed structure, so it can be employed to evaluate local properties, as particle center distribution, radial and axial void fraction profile, number of particles contacting lateral wall and co-ordination number. These results are being currently analyzed and will be reported in due time.

It is worth remarking that real spherical packing will usually presents some dispersion in particle size. The algorithm presented here could be readily extended to analyze a mixture of spheres of different diameters.

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