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CFD-based analysis of the wall effect on the pressure drop in packed beds with moderate tube/particle diameter ratios in the laminar flow regime

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ABSTRACT

In this work, the influence of the confining walls on pressure drop in packed beds is studied numerically for moderate tube/particle diameter ratios. Two different configuration types are investigated, a regular type and an irregular one. The regular configurations follow the atomic body-centered cubic and face-centered cubic structure in ideal crystals, whereas the modified ballistic deposition method is employed to generate the irregular configurations. To validate the simulation results, four experimental pressure drop correlations are used, namely by Ergun (1952) [1], by Carman (1937) [2], by Zhavoronkov et al. (1949) [3] and by Reichelt (1972) [4]. Simulation results for the regular configurations are in a good agreement with the Carman correlation. For the irregular configurations, which are closer to real packed beds, agreement with the correlations of Zhavoronkov et al. (1949) [3] and Reichelt (1972) [4] is better. This is explained by the fact that the latter two correlations take the wall effect into account. CFD simulations provide useful data on the flow field inside packed beds which can be used for the improvement and further optimization of the design and operation of packed bed reactors.

1. Introduction

Packed bed reactors have been widely used in numerous industrial applications for more than 70 years. They are applied in different chemical processes, such as gas absorption, stripping and catalytic conversion. Although new structured catalysts and reactors have been developed, packed bed reactors will most probably be still in use in the forthcoming decades, mainly because of their low cost [5].

Pressure drop is of crucial importance for the design and operation of packed bed reactors. There are several works, both experimental and numerical, approaching a correct description of the pressure drop in packed beds.

A review on the influence of the confining walls on the pressure drop in packed beds was published by Eisfeld and Schnitzlein [6], whereas experimental data mainly found in the literature were compared with a number of correlations. In their investigations, Reichelt's approach was found to be the most promising for the prediction of the pressure drop since it showed the smallest deviation from the experimental data for a wide range of Reynolds numbers ($0.01 \leq Re_p \leq 17{,}635$) and different packed bed configurations (tube/particle diameter ratios of $1.624 \leq \lambda \leq 250$ and average bed porosity $0.330 \leq \bar{\varepsilon} \leq 0.882$).

Two different numerical approaches can be found in literature to describe the hydrodynamic and transport properties of packed beds. In the first one, packed beds are treated as a pseudo-homogeneous media, where modified Navier–Stokes equations are applied in conjunction with the Ergun pressure drop correlation to account for the fluid–solid interaction [e.g., 7–11]. To govern local phenomena, overall averaged quantities are replaced by functions describing the radial change of these quantities. For example, to account for the radial porosity variation, the overall averaged porosity of the whole packed bed reactor is replaced with a function accounting for the porosity distribution along the reactor radius. Different empirical correlations have been developed for the radial porosity profiles [9,12,13], and their application may result in large differences in the radial porosity profiles, especially in the case of packed beds with moderate tube/particle diameter ratios, thus leading to substantially different radial velocity profiles.

In the second approach, the packed bed is simulated based on the consideration of the actual packed bed geometry. This yields a detailed description of the liquid flow between the particles. In this way, no additional empirical correlation is required for the porosity distribution. To resolve the fluid flow between particles, two different methods are used. The first one is the lattice Boltzman method (LBM). Using the LBM, Freund et al. [14] calculated the local velocity and the pressure drop in irregular arrangements of spheres in cylindrical containers and the simulation results were in a good agreement with experimental data. In the second method, the Navier–Stokes equations are applied to the void between the spheres. In the work of Calis et al. [5], the local velocity field in

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Nomenclature

d_p	particle diameter (m)
D	tube diameter (m)
L	length of the packed bed (m)
ΔP	pressure drop (Pa)
r	radial position (m)
Re_p	$d_p \rho U_0/\mu$, particle Reynolds number, dimensionless
u	radial average velocity (m/s)
U_o	superficial velocity (m/s)
z	$(D - r)/d_p$, distance from wall, dimensionless

Greek letters

ε	radial porosity, dimensionless
$\bar{\varepsilon}$	average porosity, dimensionless
ε_{inf}	bed porosity of infinite in diameter packed beds, dimensionless
λ	tube/particle diameter ratio, dimensionless
μ	dynamic viscosity (Pa s)
ρ	density (kg/m^3)
ψ	dimensionless pressure drop

both regular and irregular configurations of spheres was studied in rectangular containers for tube diameter/particle diameter ratio up to four. Furthermore, Dixon and Nijemeisland [15] investigated the relationship between the local flow field and the local wall heat flux in a packed bed of spheres. Klöker et al. [16] studied the mass transfer phenomena for different flow rates in arranged spherical geometries.

Our objective is to study the influence of the confining walls on the pressure drop in different packed bed configurations with the aid of computational fluid dynamics (CFD). Pressure drop values obtained numerically for different flow rates are compared with experimentally derived correlations from the literature.

2. Geometries studied

In this work, two different particle configuration types are studied, a regular and an irregular one. The regular configurations follow the atomic body-centered cubic (BCC) and face-centered cubic (FCC) structure in ideal crystals. To build the irregular packed bed configuration of non-overlapping spherical particles, a ballistic deposition method is employed [17]. This method is modified by means of the Monte Carlo approach. In order to place one spherical particle inside a tube, a relatively large number of “test” particles are dropped, and only the particle with the lowest final position becomes a part of the stack. In Fig. 1, the total number of bed particles and the average bed porosity are plotted against the number of “test” particles. If the number of “test” particles, N, is high enough ($N > 10^6$), random arrangements can be generated. This method results in irregular configurations similar to those obtained with the most rigorous ballistic deposition algorithms, while requiring significantly less computational time and programming work complexity [18].

The tube diameter/particle diameter ratio for the geometries studied in our work lies between 1 and 7. For this range of ratios, the wall effect on the pressure drop is significant [10].

3. Model description and implementation

For the description of the complex 3D flow field between the particles inside a packed bed reactor, the momentum and continuity equations were used. The flow within the packed bed was considered incompressible and steady-state. The solid particles did not move and the void between them remained constant. All simulations were performed for the laminar flow regime ($Re_p < 100$), since in this regime pressure drop changed significantly with the particle Reynolds number and large variations were expected.

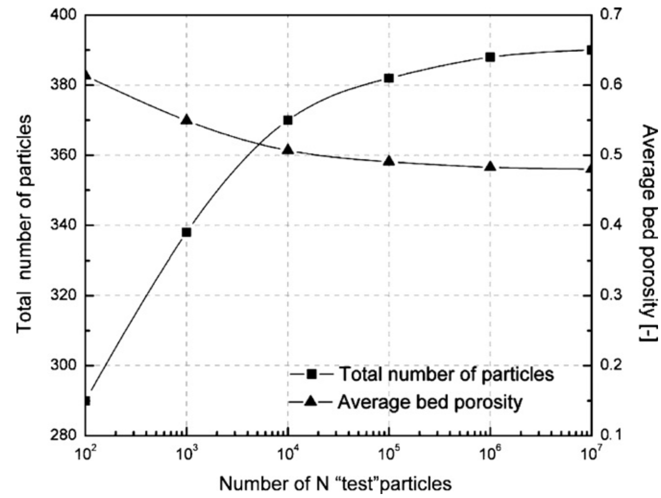

Fig. 1. Total number of particles and average bed porosity as functions of the number of “test” particles.

Due to the complex geometry, an unstructured tetrahedral grid was used for an appropriate discretization of the computational domain. To avoid low-quality mesh elements at the contact points particle/particle and particle/confining wall, all particles were shrunk by 2% of their diameter after the bed generation. In the ballistic deposition method, we used particles of 1 mm diameter. Before meshing, the diameter of each particle was reduced from 1 mm to 0.98 mm. Because of this particle diameter reduction, it was necessary to re-estimate the geometrical characteristics of the bed (average void fraction, radial porosity distribution).

During the mesh generation, special attention was paid to an accurate resolving of the boundary conditions near the particle surface where prismatic elements were used. In this work, we found that five layers of prismatic mesh elements were sufficient for the correct description of this boundary condition. To obtain grid independent results, depending on the geometrical complexity and the considered number of particles of the packed bed, up to 30 million tetrahedral and prismatic elements were used. To perform such demanding calculations, four processors (AMD Opteron MP 852-2.6 GHz) with a memory of 16 GBytes were used in parallel. In most cases, simulation time did not exceed 34 h.

To simulate the fully developed flow neglecting inlet and wall effects, periodic boundary conditions were imposed at the inlet and outlet of the domain with respect to the main flow direction. The use of periodic boundary conditions reduces the domain length resulting in a substantial reduction of the required computational power and time. This assumption was thoroughly checked and justified (see Section 4.3). At all other surfaces, the standard no-slip boundary condition was imposed.

The solution was obtained using a second-order discretization scheme. Simulations were performed with the commercial CFD software code ANSYS CFX 10.0® by ANSYS Inc.

4. Results

4.1. Analysis of the generated packed beds

All the generated packed beds consisted of monodispersed particles of 1 mm in diameter. In order to study the wall effect on pressure drop, packed beds with different tube/particle diameter ratio, both regular and irregular, were generated.

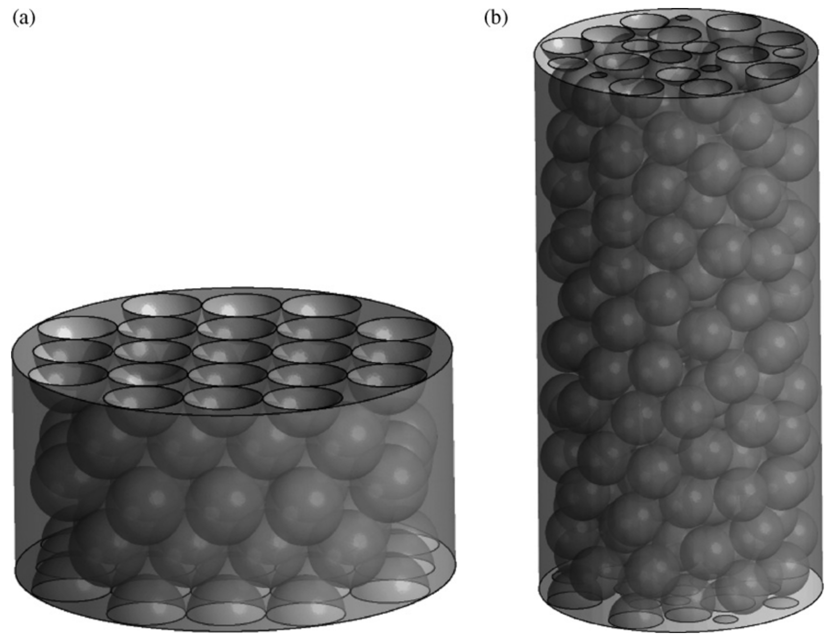

Fig. 2. Particle arrangements of the simulated regular (λ = 5.5, a) and irregular (λ = 5.0, b) configurations.

Four regular particle arrangements were constructed, with λ = 1.0 and λ = 2.68 for the BCC configuration, and with λ = 3.0 and λ = 5.5 for the FCC configuration. Since in the regular arrangements the position of each particle was fixed, it was possible to select the tube diameter in such a way that the void fraction near the confining walls was minimal. For the irregular configurations, again, four different particle arrangements were built, with λ = 2.0, 3.0, 5.0 and 7.0. In Fig. 2, the generated regular and irregular particle arrangements are shown for tube/particle diameter ratios of 5.5 and 5.0, respectively.

The first validation of the irregular geometries was done using the average void fraction of the packed beds. In Fig. 3, the average void fraction for both regular and irregular configurations is shown and compared with two experimentally determined correlations, by Jeschar [19] given by

$$\bar{\varepsilon} = 0.375 + \frac{0.34}{\lambda} \qquad (1)$$

and by de Klerk [13] given by

$$\bar{\varepsilon} = 0.41 + 0.35\exp(-0.39\lambda) \qquad (2)$$

The first correlation was developed for dense irregular packings, while the second one for loose irregular packing arrangements obtained by letting spheres just rolling loosely inside the bed. The latter way closely resembles the modified ballistic deposition method employed here for the geometry construction. As we can see, the average void fraction of the generated irregular geometries is higher compared to both correlations. This can be attributed to the average void fraction increase caused by the shrinking procedure used in our work to avoid low-quality mesh elements.

In Fig. 4, the radial porosity distribution for a regular (λ = 5.5) and irregular (λ = 5.0) geometry is shown. These radial distributions are compared with the experimentally determined correlation given

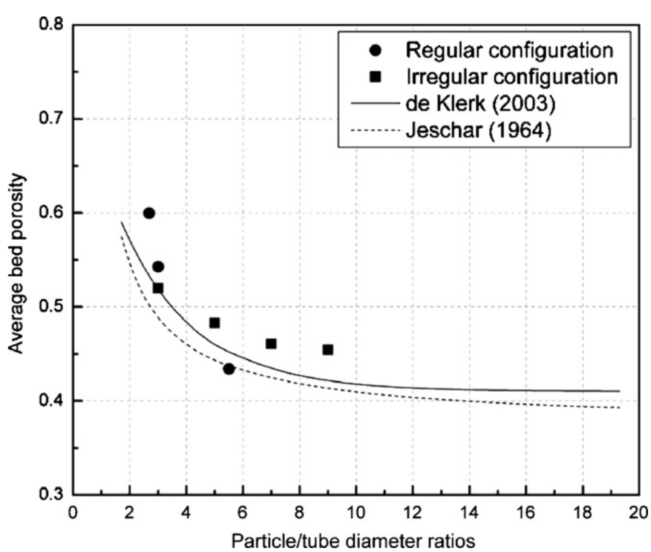

Fig. 3. Average porosity of the generated packed beds as a function of tube/particle diameter ratio.

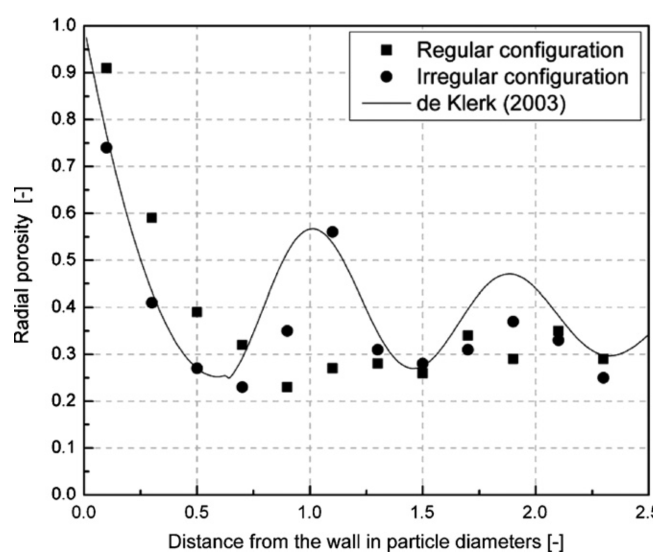

Fig. 4. Radial porosity of the simulated regular (λ = 5.5) and irregular (λ = 5) configurations.

by de Klerk [13]:

$$\varepsilon(r) = \begin{cases} 2.14z^2 - 2.53z + 1, & z \le 0.637 \\ \varepsilon_{\text{inf}} + 0.29\exp(-0.6z)[\cos(2.3\pi(z-0.16))] + 0.15\exp(-0.9z), & z > 0.637 \end{cases} \quad (3)$$

This correlation identifies two regimes, one close to the wall and one far from it. As mentioned by de Klerk [13], the correlation is able to describe accurately the porosity variations near the confining wall, while, far from the wall, it leads to higher bed porosities than in experiments. This is mainly due to the application of a periodic (cosinusoidal) description of the porosity oscillations.

Radial void fraction profile of the constructed regular geometries is completely different from that given by the de Klerk [13] correlation. The minimum void fraction is approximately one particle diameter away from the wall and the profile remains almost constant at higher distances from the wall. On the contrary, the radial porosity distribution of the irregular configuration is in a good agreement with the de Klerk [13] correlation up to a distance of 1.5 particle diameters from the wall. The first layer of particles in contact with the wall is highly ordered resulting to a minimum void fraction at approximately half particle diameter from the wall. Another minimum can be observed at a distance of 1.5 particle diameters. On the other hand, at higher distances from the wall, the porosity estimated using the ballistic deposition method is lower compared to that given by the de Klerk [13] correlation, which overestimates the porosity far from the wall.

It is thus clear that numerical solution using the modified ballistic method yields a representative geometrical description of a packed bed reactor which can be applied for CFD simulations. Additionally, this method helps to estimate radial void fraction distribution for different tube/particle diameter ratios. Such distributions can assist in significant improvement of our understanding of the packed bed configuration and, consequently, in reducing the inaccuracy in existing empirical correlations.

4.2. Grid independency study

As a first step of all simulations, a grid independency study was performed. In Fig. 5, the vertical velocity distribution as function of the radius at the half of the packed bed height is shown for $\lambda = 7.0$. Particles are located at the places where zero velocities are observed. To reach grid independent results, about 30 million tetrahedral and prismatic mesh elements were necessary. We found that five layers of prismatic mesh elements were required to resolve accurately the wall boundary condition at each particle surface. The absence or the use of smaller number of these prismatic elements led to non-physical velocities exactly on the surface of the particles. Therefore, within the void between two particles, 10 prismatic elements and at least 2 tetra elements were necessary for the proper discretization of the computational domain. The total thickness of the prismatic elements layer was 0.02 mm, whereas the thinnest layer was close to the particle surface and each further layer was expanded by a factor of 1.2.

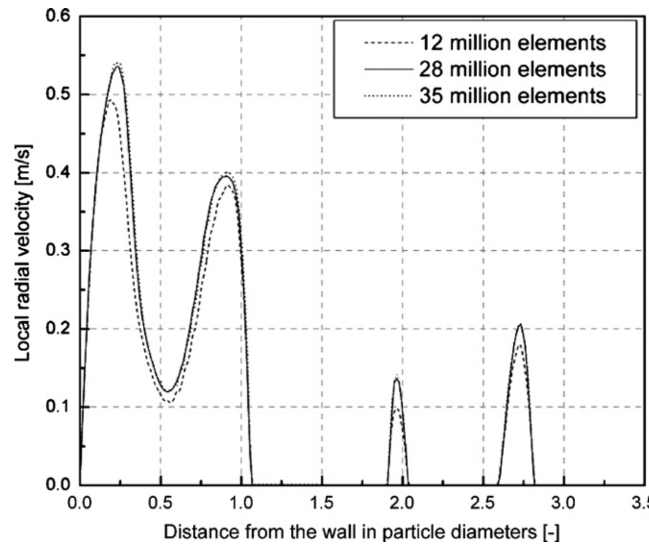

Fig. 5. Vertical velocity distribution at the half of the packed bed reactor for the irregular geometry ($\lambda = 7.0$) for different numbers of mesh elements.

4.3. Influence of the periodic boundary condition

In all simulations, periodic boundary conditions with respect to the main flow direction were used. In order to examine the influence of this assumption on the flow within the packed bed,

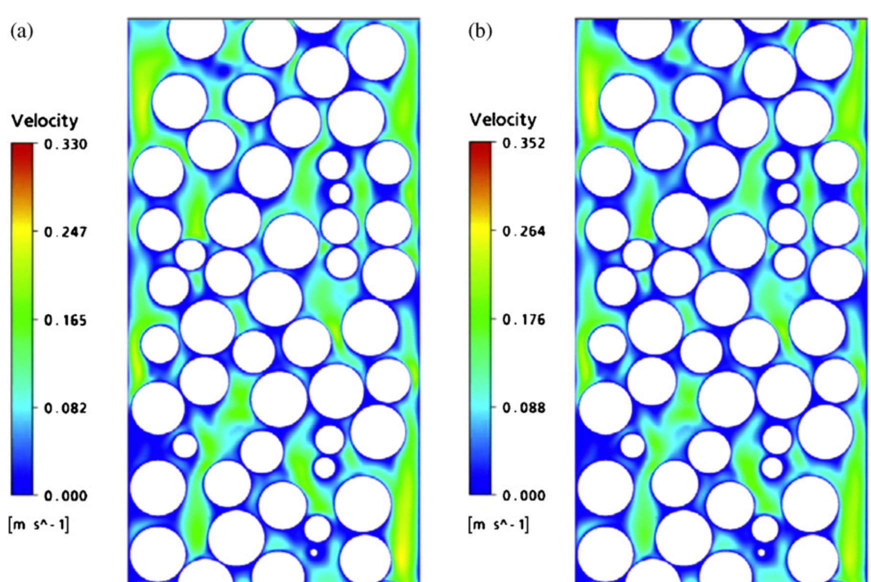

Fig. 6. Velocity distributions in the middle of the packed bed reactor obtained with common inlet/outlet boundary conditions (a) and with periodic boundary conditions (b) for $Re_p = 36.96$.

Table 1
Pressure drop characteristics.

	Equation	Constants	Wall correction	Relative root mean square deviation (spheres)
Carman [2]	$\psi = \frac{6^{3-n}k}{\mathrm{Re}_p^{2-n}} \frac{(1-\bar{\varepsilon})^{3-n}}{\bar{\varepsilon}^3}$	$n=1, k=5$	No	0.1889
Ergun [1]	$\psi = \frac{A}{\mathrm{Re}_p} \frac{(1-\bar{\varepsilon})^2}{\bar{\varepsilon}^3} + B \frac{1-\bar{\varepsilon}}{\bar{\varepsilon}^3}$	$A=150, B=1.75$	No	0.1905
Zhavoronkov et al. [3]	$\psi = \frac{A}{\mathrm{Re}_p} \frac{(1-\bar{\varepsilon})^2}{\bar{\varepsilon}^3} + B \frac{(1-\bar{\varepsilon})}{\bar{\varepsilon}^3}$	$A = 165.35 A_\mathrm{w}^2, B = 1.2 B_\mathrm{w}, A_\mathrm{w} = B_\mathrm{w} = 1 + \frac{1}{2(D/d_\mathrm{p})(1-\bar{\varepsilon})}$	Yes	0.1805
Reichelt [4]	$\psi = \frac{K_1 A_\mathrm{w}^2}{\mathrm{Re}_p} \frac{(1-\bar{\varepsilon})^2}{\bar{\varepsilon}^3} + \frac{A_\mathrm{w}}{B_\mathrm{w}} \frac{1-\bar{\varepsilon}}{\bar{\varepsilon}^3}$	$K_1 = 154, A_\mathrm{w} = 1 + \frac{2}{3(D/d_p)(1-\bar{\varepsilon})}, B_\mathrm{w} = \left[k_1 \left(\frac{d_\mathrm{p}}{D}\right)^2 + k_2\right]^2, k_1 = 1.15, k_2 = 0.87$	Yes	0.1684

simulations were performed using both periodic and standard inlet/outlet boundary condition for the same particle Reynolds numbers. In Fig. 6, the flow field in the middle of the packed bed reactor is presented. The results are obtained with both types of boundary conditions for a particle Reynolds number of 36.96. Small deviations can be observed only near the inlet; otherwise, the computational domain velocities are similar. The pressure drop difference was found to be approximately 1%.

In a strict sense, the use of periodic boundary conditions introduces some discrepancy; however, it helps to reduce computational power and time. The small observed deviation near the inlet of the computational domain does not have significant influence on the estimation of the pressure drop. Furthermore, no influence of the periodic boundary conditions on the packed bed randomness is noticed, mainly because the packed bed is generated by the ballistic deposition method. The randomness of the packing depends on the geometry generated rather than on the boundary conditions used.

4.4. Pressure drop

To validate the CFD-based approach, the pressure drop is calculated and compared with the most widespread correlations, namely, by Carman [2], Ergun [1], Zhavoronkov et al. [3] and Reichelt [4]. A comparison of these correlations is given by Eisfeld and Schnitzlein [6]; their characteristics are summarized in Table 1. The correlations by Zhavoronkov et al. [3] and Reichelt [4] take the influence of the wall into account.

In all simulations, water at 20 °C is used as a fluid medium. In Fig. 7, the pressure drop simulation results are compared with the results obtained using the four correlations for similar tube diameter/particle diameter ratio, for both regular and irregular configurations. The dimensionless pressure drop is determined as follows:

$$\psi = \frac{\Delta P}{L} \frac{d_\mathrm{p}}{\rho U_0^2} \qquad (4)$$

For the regular configurations, we used an additional correlation, developed by Susskind and Becker [20] for geometrically ordered packed beds. In this correlation, the effect of the confining walls is taken into account. Simulation results on pressure drop for the regular packing configuration agree better with the correlation of Susskind and Becker [20] than with the other correlations for the pressure drop used in our work. At the regular geometries, high local velocities are observed near the wall due to significant local void fraction there. Such high near-wall local velocities were also observed in experimental investigations (cf. e.g., [9]) being known as the wall effect or channeling. Channeling in regular packing configurations is available throughout the entire bed, resulting in a lower pressure drop than that of an irregular packed bed with the same average void fraction. For this reason, the correlations by Ergun [1], Zhavoronkov et al. [3] and Reichelt [4] developed for irregular particle configurations yield higher pressure drop values than those of the regular configurations. The correlation by Carman [2] predicts pressure drop well for small particle Reynolds numbers. However, for higher particle Reynolds numbers, this correlation yields underestimated values, because it does not account for inertia effects.

For the irregular geometry, simulation results agree better with the correlations that take into account the wall influence. The void fraction near the wall is here lower than in the regular configuration significantly reducing the near-wall channeling. Channeling in the irregular configuration is observed at regions with high local void fraction, both near the wall and inside the packing. The irregular spherical packing configuration is closer to the actual packed bed, and hence, the bed irregularities should be taken into account for the correct pressure drop description.

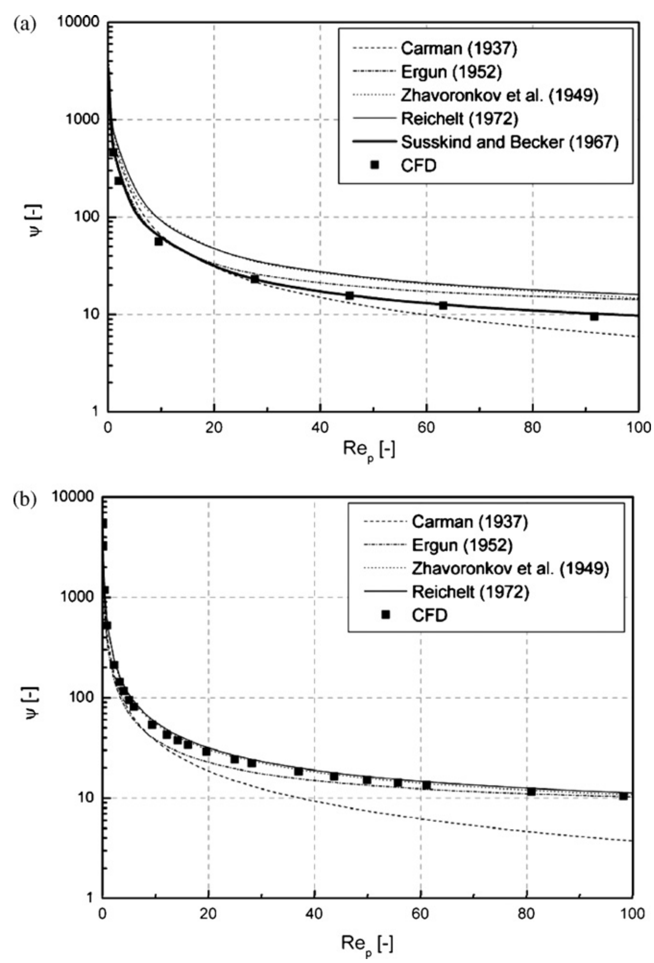

Fig. 7. Dimensionless pressure drop calculated by different methods for different particle Reynolds numbers, Re_p, for the regular ($\lambda = 5.5$, a) and random ($\lambda = 5$, b) configurations.

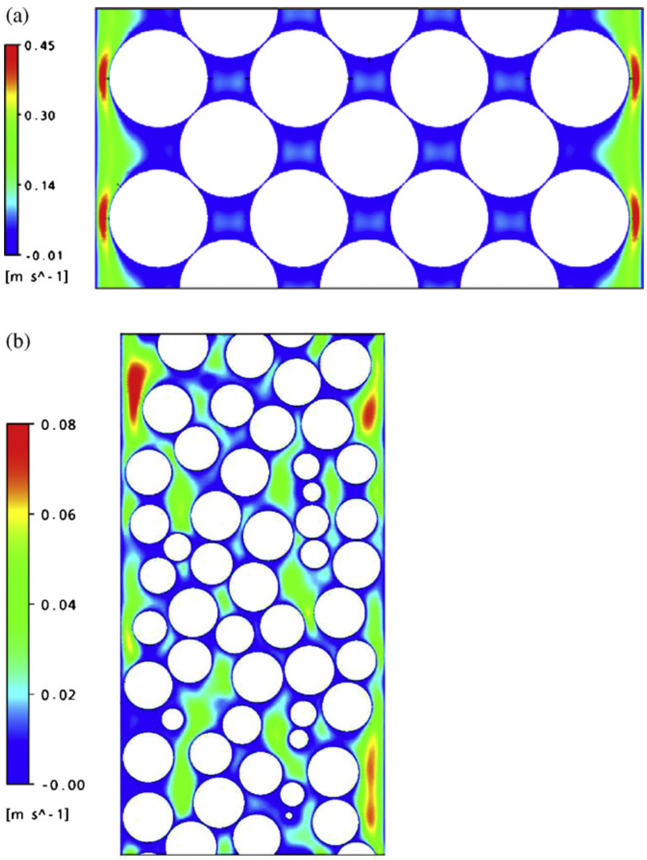

Fig. 8. Velocity distribution in the middle of the packed bed reactor for the regular ($\lambda = 5.5$, a) and irregular ($\lambda = 5$, b) configurations for $Re_p = 63$.

4.5. Velocity profiles

In Fig. 8, the flow field is presented for the regular and irregular geometry for particle/tube diameter ratios of 5.5 and 5.0, respectively, and for a particle Reynolds number of 10. For the regular geometry, high velocities are observed in the region near the confining wall where the void fraction is high. On the contrary, in the inner tube region, velocities are almost zero since the local void fraction is very low.

For the irregular geometry, channeling is not as structured as in the regular one. In this case, channeling is mainly observed near the wall where local void fraction is higher, but it also appears in the inner regions of the packing. Local velocities near the wall are approximately 8 times higher than the superficial velocity; on the other hand, behind the particles, zero velocity areas can be observed.

In Fig. 9, the velocity distribution in two cross-sections of the packed bed reactor distanced by half of a particle diameter is shown. Since the geometry changes substantially, the velocity distribution changes as well. Based on these local velocities, radial average velocity profiles can be obtained by integrating the local velocities over a sufficiently thin area between two circumferences with the radii $r - \Delta r$ and $r + \Delta r$. Δr is decreased until the calculated radial average velocities are independent of its value. The presence of solid particles within this area is taken into account by zero velocity values inside them. In Fig. 10, the average radial profiles are plotted as a function of the distance from the wall measured in particles diameters. For both plotted profiles, we can observe a similar oscillating behavior held up to 1.5 particle diameters from the wall. Radial average velocity is equal to zero exactly at the wall. The first velocity maximum is reached at approximately one-fourth of

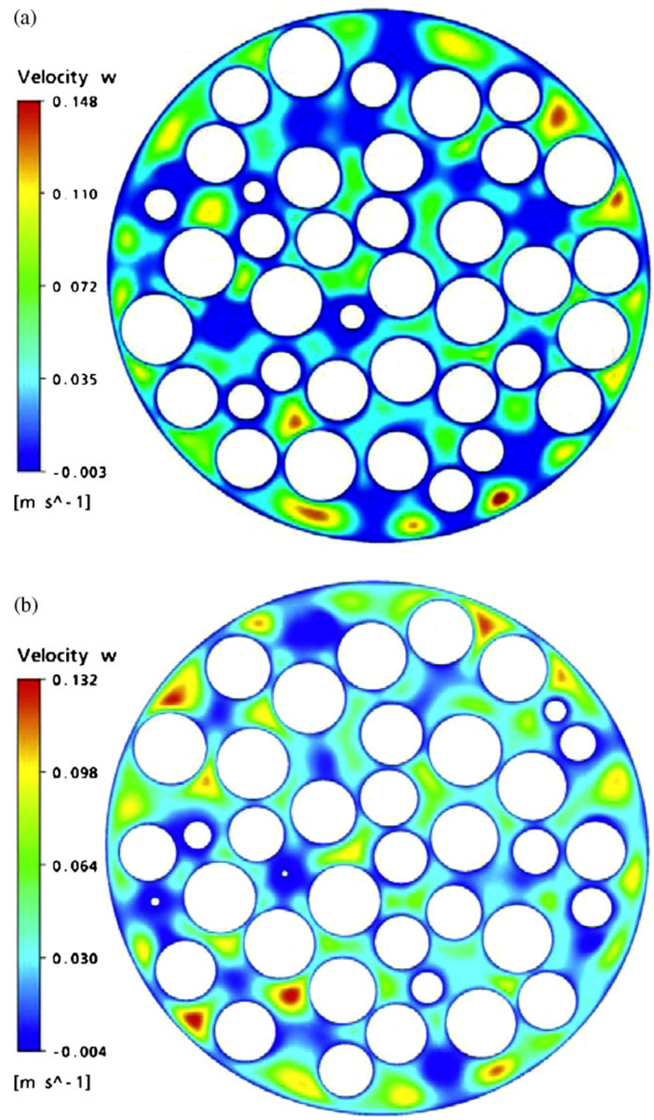

Fig. 9. Velocity distribution for $\lambda = 7$, $Re_p = 20$, $U_o = 0.019$ m/s at a bed length of 1.0 cm (a) and 1.05 cm (b).

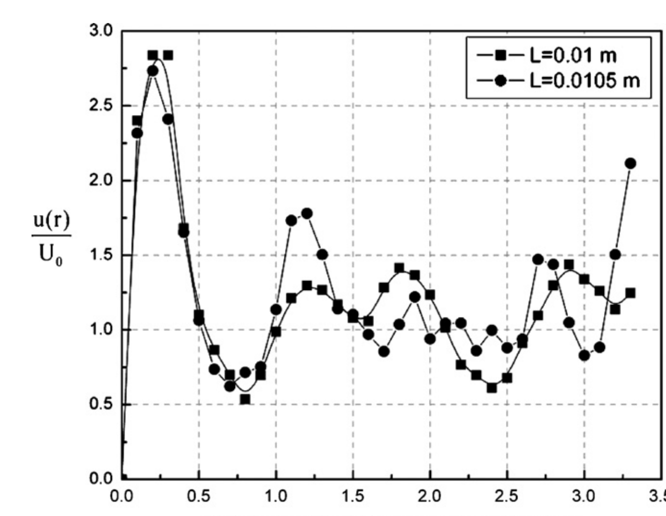

Fig. 10. Average velocity distribution as function of the reactor radius for $\lambda = 7$, $Re_p = 20$, $U_o = 0.019$ m/s at different lengths of the packed bed reactor.

the particle diameter from the confining wall and it is 2.5–3 times higher than the superficial velocity. A second peak appears at a distance of one particle diameter from the wall. This behavior of the average radial velocity profiles is quite typical and has been observed in both experimental and numerical studies found in the literature [e.g., 9,14]. Particles near the wall are highly ordered, and thus, these oscillations are to be expected. As the distance from the wall increases (higher than 1.5 particle diameters), the regularity of the particle configuration drops and larger deviations from the oscillatory behavior are to be expected, depending on the packed bed geometry.

In general, large velocity variations can be identified even within small distances (less than half of a particle) due to extensive change of the bed geometry in the direction normal to the flow. In a number of works [e.g., 9–11], in which fixed beds are modeled using the pseudo-homogeneous approach, the radial-averaged velocities profiles are assumed to be constant along the axial direction of packed bed for low or moderate tube/particle diameter ratios, since the local porosity varies only with respect to the radial coordinate. As we have shown, due to the large variations of the packed bed geometry in the axial direction, these radial profiles within a fixed bed reactor are not at all constant, and in many cases, the averaged velocity is substantially lower than the real local velocity. This can result in large errors in the simulations with the pseudo-homogeneous approach, especially in the case when mass and heat transfer phenomena become important.

5. Conclusions

In this work, the influence of confining walls on pressure drop in regular and irregular beds of spheres is studied using CFD. Different bed configurations with different tube/particle diameter ratios are generated. In all simulations, inlet effects are neglected and periodic boundary conditions in the main flow direction are applied.

For the generation of the irregular packing configuration of non-overlapping spherical particles, a ballistic deposition method is employed in combination with the Monte Carlo method. This method results in representative irregular particle configurations.

Numerical investigations of the regular configurations show strong channeling throughout the bed near the wall where the local void fraction is substantially high. The flow inside the packing is very slow. For the irregular geometry, channeling is not as structured as for the regular one. It is mainly observed near the wall, but also partly exists in the inner regions of the packing.

To validate the simulation results, experimentally determined pressure drop correlations are used. Numerical results for the irregular configuration agree better with the correlation by Zhavoronkov et al. [3] and Reichelt [4] in which the wall effect on pressure drop is taken into account.

Radial average velocity profiles are estimated using the local velocities. Our study shows that the radial profiles are not constant along a packed bed reactor with moderate tube/particle diameter ratio, and in many cases, the averaged velocity is substantially lower than the real local velocity. Within the pseudo-homogeneous approach, these profiles are assumed constant along the packed bed. This assumption may lead to errors for moderate tube/particle diameter ratios. Thus, rigorous CFD simulations are proven to be useful for identification of the drawbacks of simplified semi-empirical modeling approaches and for their further improvement by developing better empirical correlations. The developed CFD-based approach provide knowledge that often is difficult to obtain experimentally and can contribute to improving the design of moderate tube/particle diameter ratio packed beds. Furthermore, CFD simulations can be easily extended to account for mass and heat transfer phenomena.

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