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Experimental and Numerical Investigation of Structure and Hydrodynamics in Packed Beds of Spherical Particles

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In chemical industry, flows often occur in nontransparent equipment, for example in steel pipelines and vessels. Magnetic resonance imaging is a suitable approach to visualize the flow, which cannot be performed with classical optical techniques, and obtain quantitative data in such cases. It is therefore a unique tool to noninvasively study whole-field porosity and velocity distributions in opaque single-phase porous media flow. In this article, experimental results obtained with this technique, applied to the study of structure and hydrodynamics in packed beds of spherical particles, are shown and compared with detailed computational fluid dynamics simulations performed with an in-house numerical code based on an immersed boundary method-direct numerical simulation approach. Pressure drop and the radial profiles of porosity and axial velocity of the fluid for three packed beds of spheres with different sizes were evaluated, both experimentally and numerically, in order to compare the two approaches. © 2018 The Authors AIChE Journal published by Wiley Periodicals, Inc. on behalf of American Institute of Chemical Engineers

Keywords: packed bed, magnetic resonance imaging, discrete element method, immersed boundary method, direct numerical simulation

Introduction

One of the most common reactors in chemical industry is the packed bed reactor, in which the fluid phase flows through a fixed bed of solid particles. In many applications, the solid particles are catalyst pellets. The performance of a packed bed as a chemical reactor is closely related to the nonuniformity of the flow. Therefore, detailed modeling using computational fluid dynamics (CFD) as well as noninvasive monitoring of packed beds is receiving increased attention. Before the introduction of tomography and magnetic resonance imaging (MRI), only overall properties of a packed bed could be determined, for example integral flow rates, pressure drop, liquid holdup, wetting efficiency, axial dispersion, and residence time distribution. Even though global properties of the hydrodynamics are useful, they are usually not sufficient to predict the performance of the reactor, since the inhomogeneity of the packing structure causes significant local variations in holdup, wetting, and fluid velocities.

Apart from imaging the fluid distribution in the bed, MRI allows to acquire noninvasive measurements of the local fluid velocities. These data can be used to check for the accuracy and appropriateness of assumptions used in numerical modeling of packed beds. In a general review on MRI applied to chemical engineering, Gladden and Sederman show that flow rates from microns per second up to meters per second can be measured, and time scales of measurement are just a few milliseconds. The data acquisition rates that can be achieved are, for some systems, competitive with those obtained by laser-based velocimetry, but MRI has the important advantage that it can be used in optically opaque systems, which is the main reason to use MRI when investigating three-dimensional (3-D) systems.

Many studies on structure and hydrodynamics in packed beds are based solely on simulations. Gunjal et al. studied single-phase flow through an array of spheres using the unit-cell approach, in which different periodically repeating arrangements of particles were considered. The model was first
validated with published experimental and computational results and then used to study the effect of particle arrangement and orientation on velocity distribution. The simulated results were also used to quantify relative contributions of surface drag and form drag in overall resistance to the flow through packed bed reactors. Atmakidis and Kenig used a commercial software package (ANSYS CFX) to study the flow in a regular and an irregular configuration of spherical particles with different column-to-particle diameter ratios. They generated the irregular packing configuration with a ballistic deposition method and obtained average radial porosity and axial velocity profiles, showing that in many cases the average axial velocity is substantially lower than the real local velocity. Following a similar approach, Boccardo et al. employed an open-source workflow based on coupling Blender software, for the generation of random packings of particles with different shapes, with OpenFOAM for CFD simulations, obtaining results for porosity and velocity distributions inside the packed bed. Concerning the effect of particle shape, Dorai et al. performed fully resolved simulations of the flow through packed beds of monodisperse and polydisperse systems of spherical and cylindrical pellets in the viscous regime, showing that a correlation for polydisperse spheres can be used also for cylinders of moderate aspect ratio.

Extensive research has been done on MRI applied to packed beds. Sederman et al. used MRI to probe structure-flow correlations within the interparticle space of a packed bed of balloons. Images of the three mutually orthogonal components of the velocity field were obtained in two perpendicular slices. A comparison of flow images obtained for two beds of identical column-to-particle diameter ratio and different length showed that velocity enhancements at the walls of the bed were greater in the shorter bed. A 3-D volume image of each bed was also obtained and analyzed to partition the interparticle space into individual pores and determine the location of pore necks. It was found that, for pores associated with low local Reynolds number, the volume flow rate through the constrictions scales as the square of the cross-sectional area of the constriction, whereas at the extreme of high local Reynolds number pores show volume flow rates scaling with cross-sectional area. Sederman and Gladden presented results for 3-D MRI and flow visualization applied to single and two-phase flows occurring within packed beds of glass spheres. Visualization of air-water flow was also reported, and the capability of MRI to yield information on rivulet formation and surface wetting features was illustrated. Sederman et al. used MRI volume-visualization in combination with image analysis techniques to characterize the structure within the interparticle space of unconsolidated and consolidated packed beds. The beds were characterized using two approaches. First, radial distributions of the voidage were calculated. The reduced radial distribution function of the void space in a plane perpendicular to the axis of the bed was also used to investigate correlated structures within the void space. Second, the interparticle space was segmented into individual pores, defined as a portion of the void space bounded by a solid surface and planes located at positions where the hydraulic radius of the void space exhibits a local minimum. Statistical distributions of the features of these pores, such as radius, surface area, volume, and coordination to other pores, were obtained. Ren et al. combined different magnetic resonance techniques to obtain information on structure and velocity for packed beds with low column-to-particle diameter ratio. The structure of the void space was determined for glass beads arranged in regular and irregular configurations. By combining MRI with velocity encoding, velocity profiles and distributions of flow velocity components of a single fluid phase through packed beds were acquired. Using the same principles, Sankey et al. imaged both the gas and liquid velocities during stable liquid-gas flow of water and pressurized sulfur hexafluoride within a packing of spheres in a trickle bed. Liquid and gas flow rates, calculated from the velocity images, were found in agreement with macroscopic measurements. In addition to the information obtained directly from these images, the ability to measure liquid and gas flow fields within the same sample environment enabled them to explore the validity of assumptions used in numerical modeling of two-phase flows.

In available literature, there are some scientific publications where MRI findings are compared with CFD simulations, often based on the lattice-Boltzmann technique or on commercial codes (some examples can be found in Manz et al., Mantle et al., Robbins et al., and Yang et al.). A detailed comparison between DNS simulations and Particle Image Velocimetry (PIV) data was made by Wood et al., but in this case the experimental method was limited to a 2-D system (a single plane within the porous medium). In the present work an in-house code, based on the immersed boundary method-direct numerical simulation (IBM-DNS) numerical approach, is used for a comparison with experiments. Where Lattice-Boltzmann methods and body-fitted meshes are limited in use for dense particle systems including mass and heat transport, the IBM-DNS can be more straightforwardly used and this represents a breakthrough with respect to previous studies. Experimental results of MRI applied to packed beds of spherical particles are compared with detailed IBM-DNS simulations on a one-to-one basis, which will serve as a first hydrodynamic basis for further studies. Liquid water has been chosen as a suitable fluid for experimental investigations, since it contains $^1$H nuclei, and nuclear spin densities in the liquid phase are almost 1000 times higher than those in the gas phase.

In this article, a description is given on how MRI principles can be applied to reconstruct the position of particles in experimental packed beds and to evaluate the axial velocity of water flowing through them. Experimental results have been compared with detailed CFD simulations, revealing that the validation of numerical codes is possible when accurate datasets are acquired using MRI.

To complete the hydrodynamic characterization of the system studied, pressure drop has been evaluated through

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**Figure 1. Scheme of the experimental setup used to perform experiments.**

The MRI scanner is horizontal. [Color figure can be viewed at wileyonlinelibrary.com]
experiments and CFD simulations and results have been compared with available literature correlations (Eisfeld and Schnitzlein\textsuperscript{16} and Macdonald et al.\textsuperscript{17}).

Materials and Methods

Three packed beds of monodisperse polypropylene spheres ($d = 3, 4,$ and $5 \pm 0.05 \text{mm}$) were arranged in a polycarbonate (Lexan) cylinder ($D = 21 \text{mm}, L = 61 \text{mm}$). Liquid water, pumped from a reservoir by means of a peristaltic pump (Watson-Marlow Qdos60 Universal) at flow rates corresponding to particle Reynolds numbers ($Re_p = \frac{\rho U_0 d}{\mu}$) of 10 and 50, was distributed into the beds through a porous glass frit with 90 $\mu$m pores. A dampener was placed on the discharge line of the pump to avoid pulsating flow in the closed hydraulic circuit used to recirculate water. The whole experimental setup, operating at atmospheric pressure and ambient temperature (20°C), is shown in Figure 1.

The small Lexan column was mounted on a plastic holder and therefore placed in the bore of a 9.4 T horizontal MRI scanner (Bruker BioSpin, Ettlingen, Germany). The central section of the column, measured along the axial direction, was aligned with the isocenter of a $^1\text{H}$ quad transceiver coil with an inner diameter of 35 mm and images were acquired by means of standard methods available with ParaVision 5.1 software (Bruker BioSpin, Ettlingen, Germany). Prior to image acquisition, matching and tuning of the coil was performed.

A 3-D FLASH sequence [echo time (TE): 6 ms, repetition time (TR): 15 ms, flip angle (FA): 5°, field of view (FOV): $25 \times 25 \times 25 \text{mm}^3$, matrix of voxels (MTX): $128 \times 128 \times 128$, resolution (RES): $0.195 \times 0.195 \times 0.195 \text{mm}^3$, number of averages (NA): 1, number of repetitions (NR): 1] was used to acquire the 3-D porous structure of the packed beds, resulting in an absolute scan time of 4.1 min for each dataset acquired. Sample slices for the three packed beds are shown in Figure 2.

A 3-D FLASH sequence called FLOWMAP (Bruker BioSpin, Ettlingen, Germany), whose details can be found in the documentation of ParaVision, was employed to directly encode the velocity of water flowing through the particles. It is a flow-compensated gradient echo method, based on a FLASH sequence, in which bipolar gradient pulses are added during the encoding period to produce a flow-dependent signal phase (Gladden and Sederman\textsuperscript{1}). The method can work in three modes (Phase Contrast Angiography, Velocity Mapping, and Fourier Flow Imaging), which differ by the number of flow encoding steps and by the reconstruction procedure. In the

![Figure 2. Sample slices, obtained with a FLASH sequence, of the packed bed structure for spheres with different diameters.](image)

Column-to-particle diameter ratio ($\lambda$) values are 7, 5.25, and 4.2 for 3, 4, and 5 mm spheres, respectively.

![Figure 3. Sample slices showing the axial velocity of the fluid directly encoded with MRI at $Re_p = 50$ for spheres with different diameters.](image)

Column-to-particle diameter ratio ($\lambda$) values are 7, 5.25, and 4.2 for 3, 4, and 5 mm spheres, respectively. [Color figure can be viewed at wileyonlinelibrary.com]
present work, the Velocity Mapping mode was used, where the resulting images represent the maps of a single velocity component. Only the component along the axial direction, \( U_z \), was encoded, being the dominant one in the direction of flow. The same parameters were used for all the packed beds studied (TE: 10 ms, TR: 50 ms, FA: 5\(^\circ\), FOV: 25 \(\times\) 25 \(\times\) 25 mm\(^3\), MTX: 128 \(\times\) 128 \(\times\) 128, RES: 0.195 \(\times\) 0.195 \(\times\) 0.195 mm\(^3\), NA: 1, NR: 1), resulting in an absolute scan time of 27.3 min for each dataset acquired. Sample slices for the three packed beds at \( R_e_p = 50 \) are shown in Figure 3. A signal threshold of 0.5\% was used to cut noise outside of flow regions (the particles and outside of the column wall) and the maximum encoded velocity of water was set to 200 and 300 mm/s for \( R_e_p \) of 10 and 50, respectively, more than sufficient to encode the maximum velocity values reached at these flow rates.

Results and Discussion

Porosity

Each experimental dataset of the porous structure, obtained using the FLASH sequence as mentioned before, was processed in MATLAB through a Spherical Hough algorithm, originally developed for biomedical imaging by Xie et al.,\(^{18}\) obtaining the 3-D position of the particles. This algorithm can detect spherical objects and, therefore, estimate their center and radius, as shown in Figure 4. Its reliability can be tested, for example, on spheres with a diameter of 3 mm, for which 313 particles were detected on an actual packed bed length of 22 mm obtaining, from simple geometrical considerations, a value of 0.42 for the average porosity of the bed. The output file, containing the positions of identified spheres, was processed with a routine developed by Das et al.,\(^{19}\) which evaluates local porosity by simply counting cells occupied by the fluid. A value of 40 grid cells per particle diameter was used, but also a value of 20 is suitable in this case, with an error of only 1\%.

Average porosity can be determined also with the correlations reported by Jeschar\(^{20}\)

\[
\varepsilon = 0.375 + \frac{0.34}{\lambda}
\]

(1)

and de Klerk\(^{21}\)

\[
\varepsilon = \varepsilon_b + 0.35e^{-0.39\lambda}
\]

(2)

where \( \varepsilon_b \) = 0.37 (Das et al.\(^{19}\)) and \( \lambda = D/d \) is the column-to-particle diameter ratio.

Experimental results were compared, in terms of porosity profiles, with those obtained for computer-generated packed beds having the same number of particles. The simulated packings were created, using the parameters shown in Table 1, with a ballistic deposition approach by means of LIGGGHTS, a discrete element method (DEM) code developed by Kloss et al.\(^{22}\) The output from this code was the 3-D position of the particles and, therefore, the same routine used for the MRI reconstructed packed beds was used to evaluate the local porosity. A comparison of the different methods used to determine the average porosity is shown in Table 2.

Table 1. Parameters Used in DEM Simulations with the LIGGGHTS Code

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle diameter (d)</td>
<td>3(\times)10(^{-3}), 4(\times)10(^{-3}), 5(\times)10(^{-3})</td>
<td>m</td>
</tr>
<tr>
<td>Column diameter (D)</td>
<td>21(\times)10(^{-3})</td>
<td>m</td>
</tr>
<tr>
<td>Number of particles</td>
<td>313, 125, 64</td>
<td>–</td>
</tr>
<tr>
<td>Particle density</td>
<td>900</td>
<td>kg/m(^3)</td>
</tr>
<tr>
<td>Young modulus</td>
<td>5(\times)10(^6)</td>
<td>Pa</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>0.42</td>
<td>–</td>
</tr>
<tr>
<td>Coefficient of restitution</td>
<td>0.66</td>
<td>–</td>
</tr>
<tr>
<td>Coefficient of friction</td>
<td>0.44</td>
<td>–</td>
</tr>
<tr>
<td>Time step</td>
<td>1(\times)10(^{-4})</td>
<td>s</td>
</tr>
</tbody>
</table>

Table 2. Comparison of Different Methods to Evaluate the Average Porosity for Packings of Spheres with Different Diameters

<table>
<thead>
<tr>
<th>Method Used for Average Porosity</th>
<th>3 mm</th>
<th>4 mm</th>
<th>5 mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \varepsilon ) (DEM, routine for porosity)</td>
<td>0.43</td>
<td>0.44</td>
<td>0.49</td>
</tr>
<tr>
<td>( \varepsilon ) (MRI, routine for porosity)</td>
<td>0.41</td>
<td>0.44</td>
<td>0.47</td>
</tr>
<tr>
<td>( \varepsilon ) (MRI, experimental ( U_b/\mu ) ratio)</td>
<td>0.41</td>
<td>0.43</td>
<td>0.46</td>
</tr>
<tr>
<td>( \varepsilon ) (CFD, numerical ( U_b/\mu ) ratio)</td>
<td>0.43</td>
<td>0.44</td>
<td>0.47</td>
</tr>
<tr>
<td>( \varepsilon ) (Jeschar correlation)</td>
<td>0.42</td>
<td>0.44</td>
<td>0.46</td>
</tr>
<tr>
<td>( \varepsilon ) (de Klerk correlation)</td>
<td>0.43</td>
<td>0.46</td>
<td>0.48</td>
</tr>
</tbody>
</table>
Radial porosity profiles, averaged along the axial direction, were obtained by integrating local porosity values over a sufficiently thin area between two circumferences with radii \( r - \Delta r \) and \( r + \Delta r \). Results for the experimental (MRI reconstructed) and simulated (generated with the DEM code) packed beds are shown in Figure 5, where they are compared also with the following correlation, obtained by de Klerk \(^{21}\)

\[
\varepsilon(s) = \begin{cases} 
  2.14s^2 - 2.53s + 1, & s \leq 0.637 \\
  
  \varepsilon_0 + 0.29e^{-0.65} \left( \cos \left( 2.3\pi(s - 0.16) \right) \right) + 0.15e^{-0.5s}, & s > 0.637 
\end{cases}
\]

where \( \varepsilon_0 = 0.37 \), \( s = (R-r)/d \) is the distance from wall in particle diameters and \( R = D/2 \) is the radius of the column.

From the comparison, it is quite clear that radial porosity profiles, even if showing the same damped oscillating response, well documented in available literature, are in good agreement only near the wall, while they differ substantially in the central part of the packed bed. This is due to the different method used to generate the packed beds. In the experimental situation, the spheres are charged in layers and pressure is exerted on them when the packed bed is arranged between the two porous disks. In simulations, performed with the DEM code, a ballistic deposition approach is used, in which particles are inserted in the column one by one (an ideal situation), and a more loose packing is generated, as can be seen from the average porosity values shown in Table 2. It can be clearly observed, however, that both the simulated and experimental profiles are able to detect the high value of porosity in the central portion of the packed bed, and this is evident especially for the case of spheres with a diameter of 5 mm, whereas the de Klerk correlation is unable to predict what actually happens.

**Pressure drop**

Pressure drop plays an important role in the design of systems involving flow through a porous medium, since it decreases with increasing particle size. In a filtration system, for example, pressure drop is crucial, because the fluid flows through the filter medium by virtue of a pressure difference across the bed. Studying pressure drop across the bed is therefore essential to determine filtration efficiency and expected time span before excessive accumulation of filtered material occurs.

From an experimental point of view, pressure drop in the packed beds of 3, 4, and 5 mm spheres was determined by excessive accumulation of filtered material occurs. Study increasing particle size. In a filtration system, for example, pressure drop correlation is the one proposed by Eisfeld and Schnitzlein,\(^{16}\) where \( A \) and \( B \) are not constants, but vary with \( \lambda \) and \( \varepsilon \). Researchers to find generalizations for \( a \) and \( b \) in terms of porosity and length scale. For creeping flow, Carman proposed a relationship among \( \lambda \), the hydraulic radius and tortuosity. For a porous medium with monodisperse spheres, Ergun proposed

\[
a = A \left( 1 - \varepsilon \right)^2 \frac{1}{\varepsilon^3 d} \quad \text{and} \quad b = B \frac{1 - \varepsilon}{\varepsilon^3} \frac{1}{d^2}
\]

where \( A = 150 \) and \( B = 1.75 \) are known as the Ergun constants. Ergun proposed this correlation for particles arranged in a very large container where wall effects are negligible. However, in the case of columns with low column-to-particle diameter ratio, the pressure drop is altered by two effects: the porosity fluctuation near the wall and the friction offered by the wall.

Macdonald et al.\(^{17}\) compared the experimental results of other authors with the Ergun correlation and proposed different values of the constants. In their studies, \( A = 180 \) for the viscous component of the pressure drop has been adopted from the Carman equation and \( B = 1.8 \) was found by fitting a large amount of experimental data, including the original results by Ergun. The authors showed that the modified Ergun correlation can describe the pressure drop with an accuracy of \( \pm 25\% \). The porosity functions, i.e., \( (1 - \varepsilon)^2/\varepsilon^3 \) for the viscous term and \( (1 - \varepsilon)/\varepsilon^3 \) for the inertial term, proposed by Ergun were found to be very accurate by several authors (Nemec and Levec\(^{23}\)) for the case of close packings. This means that, for a column with a large diameter, if different packing configurations create different porosities, the value of constants \( A \) and \( B \) should not change. For a close packing, by analytical formulation, Niven\(^{24}\) justified the use of such a porosity function for pressure drop calculations, but for loose systems this function needs to be modified. Hence, most researchers have only tried to find the values of \( A \) and \( B \) for dense packings. There is a large number of uncertainties in experimental results and, as a consequence, a huge variation can be observed in existing literature data.

The pressure gradient can be normalized as follows

\[
f = \frac{\Delta p/\Delta z}{\mu U_0/d^2} = A \left( \frac{1 - \varepsilon}{\varepsilon^3} \right) + B \frac{1 - \varepsilon}{\varepsilon^3} \frac{Re_p}{d}
\]

which shows that the pressure drop is a linear function of \( Re_p \) and the values of \( A \) and \( B \) can be found by linear regression. It is clear that, with increasing particle size, the pressure drop decreases, mainly due to the increase in the average porosity of the bed.

The pressure drop depends on bed porosity and any small variation of this quantity determines a significant change in pressure drop. To account for the wall effect, the most popular pressure drop correlation is the one proposed by Eisfeld and Schnitzlein,\(^{16}\) where \( A \) and \( B \) are not constants, but vary with \( \lambda \) and \( \varepsilon \).
Figure 5. Experimental (MRI) and simulated (DEM) radial profiles (averaged along the axial direction) of porosity for packed beds of spheres with different diameters. The continuous black line shows the correlation by de Klerk.21 [Color figure can be viewed at wileyonlinelibrary.com]

Figure 6. Scheme of the experimental setup used to measure pressure drop. [Color figure can be viewed at wileyonlinelibrary.com]

Figure 7. Experimental and numerical values of nondimensional pressure drop for different sphere sizes and the correlation of Eisfeld and Schnitzlein.16 Dashed lines indicate an error margin of 34%. [Color figure can be viewed at wileyonlinelibrary.com]

Figure 8. Experimental and numerical values of nondimensional pressure drop for different sphere sizes and the modified Ergun correlation of Macdonald et al.17 Dashed lines indicate an error margin of 25%. [Color figure can be viewed at wileyonlinelibrary.com]
This correlation fits most of the data for $k_5$ to $k_1$ with an accuracy of $\pm 34\%$. From Eq. 6, it is clear that the pressure drop constants reach a value of $A_{ES} = 154$ and $B_{ES} = 1.32$ when $k_1 \to \infty$, which are lower than the values from the Ergun or modified Ergun correlation. In Figure 7, the nondimensional pressure drop obtained from experiments and simulations is compared with the Eisfeld and Schnitzlein correlation in a log-log plot for all the packed beds. It was found that all the data lie inside the reported error band.

$$A_{ES} = 154A_{w,ES}, \quad B_{ES} = \frac{A_{w,ES}}{B_{w,ES}}, \quad A_{w,ES} = 1 + \frac{2}{3\lambda(1-\epsilon)}, \quad B_{w,ES} = \left(\frac{1.15}{\lambda^2} + 0.87\right)^2$$

(7)

This correlation fits most of the data for $\lambda = 2$ to $\lambda \to \infty$ with an accuracy of $\pm 34\%$. From Eq. 6, it is clear that the pressure drop constants reach a value of $A_{ES} = 154$ and $B_{ES} = 1.32$ when $\lambda \to \infty$, which are lower than the values from the Ergun or modified Ergun correlation. In Figure 7, the nondimensional pressure drop obtained from experiments and simulations is compared with the Eisfeld and Schnitzlein correlation in a log-log plot for all the packed beds. It was found that all the data lie inside the reported error band.

Figure 9. Sample slice perpendicular to the main flow showing the axial velocity of the fluid measured with MRI (a) and obtained from IBM-DNS (b) at $Re_p = 50$ for the same packed bed of spheres with a diameter of 5 mm.

Figure 10. Sample slice along the main flow showing the axial velocity of the fluid measured with MRI (a) and obtained from IBM-DNS (b) at $Re_p = 50$ for the same packed bed of spheres with a diameter of 3 mm. The thickness of the slice in (a) is 0.195 mm, while in (b) it is 0.075 mm. [Color figure can be viewed at wileyonlinelibrary.com]
Figure 8 shows the variation of the modified friction factor ($\psi$) with the modified particle Reynolds number ($Re_p$), as defined by Ergun:

$$\psi = \frac{\Delta p/\Delta z}{\rho U_0^2/d (1-\varepsilon)}$$  \hspace{1cm} (8)

$$Re_p' = \frac{1}{1-\varepsilon} Re_p$$  \hspace{1cm} (9)

Modified Ergun constants (Macdonald et al.\textsuperscript{17}) are used and experimental and numerical results for all the packed beds are compared with the modified Ergun equation. All the values are within ±25% with only a few exceptions.

The low column-to-particle diameter ratio determines that the pressure drop is induced by the wall shear stress and is reduced by the increase in porosity near the wall. In comparison to infinitely large columns, the overall pressure drop for the packed beds in the present study is a tradeoff between these two effects.

The differences observed between experimental and simulated values are related to velocity profiles, shown in Figure 12, and this is reflected in pressure drop evaluation, since the two variables (pressure and velocity of the fluid) are mutually linked through the Navier–Stokes equations.

**Velocity of the fluid**

From the encoded velocity values, a map of the axial velocity of the fluid can be obtained in MATLAB and compared with those from IBM-DNS simulations of the MRI.
reconstructed packed bed. A comparison for a slice perpendicular to the main flow, in the case of a packed bed with spheres having a diameter of 5 mm, is shown in Figure 9. It is clear that, even if the two maps have different spatial resolutions, the agreement is good, especially in detecting higher velocities among particles in the central part of the bed. There are only some minor differences in detecting flow near the wall, where the MRI image is affected by noise. In Figure 10, a comparison for a slice along the main flow is shown for spheres with a diameter of 3 mm. In this case, some differences between MRI and CFD are reflected both near the wall and in interstitial regions inside the bed. Some structures are also lost in the comparison, but this is due to the different resolutions used. However both the methods, even if at slightly different magnitude, are able to detect regions where axial velocity increases, for example fluid channeling near the wall at the bottom right corner of both the maps.

Experimental and numerical probability density functions (PDFs) for the axial velocity of water were obtained in MATLAB for each 3-D dataset. Only nonzero values (zero values represent the particles and the region outside the column) were considered in the computations. Results are shown in Figure 11 for all the particle sizes and flow conditions examined. Reverse flow is observed, especially in the experimental curves, and its presence is probably due to circulating flow patterns in proximity of solid surfaces or vortex-like structures at the meeting points of streamlines, as shown by Yang et al.24 and Kutsovsky et al.25

From these PDFs, average values for the axial velocity can be evaluated (Table 3), which need to satisfy the material balance on the whole bed, given by the following equation

\[ u = \frac{U_0}{\varepsilon} \]  

Concerning the CFD simulations, the in-house code implementing the IBM-DNS approach for porous media developed by Das et al.,19 based on the principles detailed in Deen et al.,26 and Deen et al.,27 was used to obtain the 3-D velocity field for the experimentally reconstructed packed beds. The input parameters are summarized in Table 4 for the three packed beds. To obtain grid independent results, a value of 40 grid cells per particle diameter was used also in this case for all the sphere sizes, which can lead to an overprediction of less than 10% for the pressure drop at \( Re_p = 50 \), as reported in Das et al.19

Radial profiles of the axial velocity of water, averaged along the axial direction, were obtained by integrating local velocity values over a sufficiently thin area between two circumferences with radii \( r - \Delta r \) and \( r + \Delta r \). The presence of solid particles within this area was taken into account by considering zero velocity values for these cells.

Table 3. Experimental and Numerical Values of the Average Axial Velocity Evaluated from the PDF Plots for Packings of Spheres with Different Diameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spheres With a Diameter of 3 mm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Computational grid</td>
<td>3×10^{-3}</td>
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</tr>
<tr>
<td>Grid size</td>
<td>7.9×10^{-3}</td>
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</tr>
<tr>
<td>Time step</td>
<td>4.4×10^{-3}</td>
<td>-</td>
</tr>
<tr>
<td>Bed diameter</td>
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<td>-</td>
</tr>
<tr>
<td>Particle diameter</td>
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<td>-</td>
</tr>
<tr>
<td>Number of particles</td>
<td>313</td>
<td>-</td>
</tr>
<tr>
<td>Fluid density</td>
<td>1.10^{10}</td>
<td>kg/m^3</td>
</tr>
<tr>
<td>Fluid viscosity</td>
<td>1.3×10^{-3}</td>
<td>Pa·s</td>
</tr>
<tr>
<td>Superficial fluid velocity</td>
<td>3.3×10^{-3}</td>
<td>m/s</td>
</tr>
<tr>
<td>Particle Reynolds number</td>
<td>10, 50</td>
<td>-</td>
</tr>
<tr>
<td>Spheres With a Diameter of 4 mm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Computational grid</td>
<td>4×10^{-3}</td>
<td>-</td>
</tr>
<tr>
<td>Grid size</td>
<td>4.10^{10}</td>
<td>m</td>
</tr>
<tr>
<td>Time step</td>
<td>4.10^{10}</td>
<td>s</td>
</tr>
<tr>
<td>Bed diameter</td>
<td>4.10^{10}</td>
<td>M</td>
</tr>
<tr>
<td>Particle diameter</td>
<td>4.10^{10}</td>
<td>M</td>
</tr>
<tr>
<td>Number of particles</td>
<td>64</td>
<td>-</td>
</tr>
<tr>
<td>Fluid density</td>
<td>1.10^{10}</td>
<td>kg/m^3</td>
</tr>
<tr>
<td>Fluid viscosity</td>
<td>1.10^{10}</td>
<td>Pa·s</td>
</tr>
<tr>
<td>Superficial fluid velocity</td>
<td>2.5×10^{-3}</td>
<td>m/s</td>
</tr>
<tr>
<td>Particle Reynolds number</td>
<td>10, 50</td>
<td>-</td>
</tr>
<tr>
<td>Spheres With a Diameter of 5 mm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Computational grid</td>
<td>5×10^{-3}</td>
<td>-</td>
</tr>
<tr>
<td>Grid size</td>
<td>5.10^{10}</td>
<td>m</td>
</tr>
<tr>
<td>Time step</td>
<td>5.10^{10}</td>
<td>s</td>
</tr>
<tr>
<td>Bed diameter</td>
<td>5.10^{10}</td>
<td>m</td>
</tr>
<tr>
<td>Particle diameter</td>
<td>5.10^{10}</td>
<td>m</td>
</tr>
<tr>
<td>Number of particles</td>
<td>64</td>
<td>-</td>
</tr>
<tr>
<td>Fluid density</td>
<td>1.10^{10}</td>
<td>kg/m^3</td>
</tr>
<tr>
<td>Fluid viscosity</td>
<td>1.10^{10}</td>
<td>Pa·s</td>
</tr>
<tr>
<td>Superficial fluid velocity</td>
<td>2.0×10^{-3}</td>
<td>m/s</td>
</tr>
<tr>
<td>Particle Reynolds number</td>
<td>10, 50</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 4. Parameters Used in IBM-DNS Simulations

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spheres With a Diameter of 3 mm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Computational grid</td>
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</tr>
<tr>
<td>Grid size</td>
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<td>M</td>
</tr>
<tr>
<td>Time step</td>
<td>1×10^{-3}</td>
<td>s</td>
</tr>
<tr>
<td>Bed diameter</td>
<td>21×10^{-3}</td>
<td>M</td>
</tr>
<tr>
<td>Particle diameter</td>
<td>3×10^{-3}</td>
<td>M</td>
</tr>
<tr>
<td>Number of particles</td>
<td>313</td>
<td>-</td>
</tr>
<tr>
<td>Fluid density</td>
<td>1.10^{10}</td>
<td>kg/m^3</td>
</tr>
<tr>
<td>Fluid viscosity</td>
<td>1.3×10^{-3}</td>
<td>Pa·s</td>
</tr>
<tr>
<td>Superficial fluid velocity</td>
<td>3.3×10^{-3}, 16.6×10^{-3}</td>
<td>m/s</td>
</tr>
<tr>
<td>Particle Reynolds number</td>
<td>10, 50</td>
<td>-</td>
</tr>
<tr>
<td>Spheres With a Diameter of 4 mm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Computational grid</td>
<td>212×212×400 = 17, 977, 600</td>
<td>-</td>
</tr>
<tr>
<td>Grid size</td>
<td>100×10^{-6}</td>
<td>M</td>
</tr>
<tr>
<td>Time step</td>
<td>1×10^{-3}</td>
<td>s</td>
</tr>
<tr>
<td>Bed diameter</td>
<td>21×10^{-3}</td>
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<td>M</td>
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<td>Number of particles</td>
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<tr>
<td>Fluid density</td>
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<td>kg/m^3</td>
</tr>
<tr>
<td>Fluid viscosity</td>
<td>1.3×10^{-3}</td>
<td>Pa·s</td>
</tr>
<tr>
<td>Superficial fluid velocity</td>
<td>2.5×10^{-3}, 12.5×10^{-3}</td>
<td>m/s</td>
</tr>
<tr>
<td>Particle Reynolds number</td>
<td>10, 50</td>
<td>-</td>
</tr>
<tr>
<td>Spheres With a Diameter of 5 mm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Computational grid</td>
<td>170×170×200 = 5, 780, 000</td>
<td>-</td>
</tr>
<tr>
<td>Grid size</td>
<td>125×10^{-4}</td>
<td>m</td>
</tr>
<tr>
<td>Time step</td>
<td>1×10^{-3}</td>
<td>s</td>
</tr>
<tr>
<td>Bed diameter</td>
<td>21×10^{-3}</td>
<td>m</td>
</tr>
<tr>
<td>Particle diameter</td>
<td>5×10^{-3}</td>
<td>m</td>
</tr>
<tr>
<td>Number of particles</td>
<td>64</td>
<td>-</td>
</tr>
<tr>
<td>Fluid density</td>
<td>1.10^{10}</td>
<td>kg/m^3</td>
</tr>
<tr>
<td>Fluid viscosity</td>
<td>1.3×10^{-3}</td>
<td>Pa·s</td>
</tr>
<tr>
<td>Superficial fluid velocity</td>
<td>2.0×10^{-3}, 10.0×10^{-3}</td>
<td>m/s</td>
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<tr>
<td>Particle Reynolds number</td>
<td>10, 50</td>
<td>-</td>
</tr>
</tbody>
</table>
The comparison between experimental values (obtained with MRI by directly encoding velocity values through the FLOW-MAP method) and CFD simulations, using the particle positions reconstructed from the MRI measurements, is shown in Figure 12. In this figure, similar behavior is observed for spheres having diameters of 3 and 4 mm, with a good agreement only near the wall. As it is apparent, while simulations are able to reproduce the general trend and the oscillating behavior of the velocity profile, it is also clear that the peaks are not well predicted, especially at increasing distances from the wall, where an underestimation can be seen with respect to experimental data, as in a similar comparison made by Boccardo et al.4

For the particular case of spheres with a diameter of 5 mm (where \( \lambda = 4.2 \)), a good agreement was achieved through the whole packed bed, since the channeling effect dominates in this case.

**Conclusions**

In this work, structure and hydrodynamics in packed beds of spherical particles with different sizes were studied using MRI and results were compared with CFD simulations, based on an IBM-DNS approach.

Structure, in terms of phase fractions and, therefore, local porosity, was reconstructed by processing, through an algorithm able to detect spherical particles, experimental 3-D datasets of the packed beds acquired with a FLASH sequence. The axial velocity of water flowing through the particles was
obtained by directly encoding velocity values via the FLOW-MAP method.

Pressure drop was evaluated through experiments and CFD simulations and results were compared with available literature correlations, showing that there is good agreement with the present study.

Data on the positions of the particles and axial velocities have been added as Supporting Information. Porosity profiles were in good agreement with simulations obtained using a DEM approach only near the wall. From the axial velocity maps, the PDFs of experimental and simulated velocity values were also obtained for each sphere size and flow condition, showing a good agreement with the overall material balance involving the relationship among average porosity, superficial and average axial velocity of the fluid. Simulated velocity profiles were found to underestimate those obtained with experiments, with the exception of spheres with a diameter of 5 mm ($\lambda = 4.2$), where the high value of porosity in the central portion of the packed bed has a dominant effect.

MRI experiments were used to validate CFD simulations with the IBM-DNS method, developed and used in recent years to perform numerical studies of transport phenomena in packed beds. Both the experimental and numerical results showed the strict relationship between velocity profiles and pressure drop, since these quantities are related through the Navière–Stokes equations.

Acknowledgments

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Notation

- $a$ = first function in pressure drop equation
- $A$ = first Ergun (or Ergun-like) constant
- $b$ = second function in pressure drop equation
- $B$ = second Ergun (or Ergun-like) constant
- $\bar{z}$ = average porosity of the packed bed
- $\bar{\zeta}$ = porosity of an infinite in diameter packed bed
- $d$ = inner diameter of the column, m
- $D$ = outer diameter of the particle, m
- $f$ = adimensional pressure drop
- $L$ = length of the column, m
- $R_e$ = Reynolds number
- $R_e_{D}$ = modified particle Reynolds number
- $s$ = distance from wall in particle diameters
- $u$ = average axial velocity of the fluid, m/s
- $U_0$ = superficial velocity of the fluid, m/s
- $z$ = axial coordinate, m

List of Abbreviations

- 3-D = three-dimensional
- CFD = computational fluid dynamics
- DEM = discrete element method
- DNS = direct numerical simulation
- FA = flip angle
- FLASH = fast low angle shot
- FOV = field of view
- IBM = immersed boundary method
- MRI = magnetic resonance imaging
- MTX = matrix of voxels
- NA = number of averages
- NR = number of repetitions
- PDF = probability density function
- RES = resolution
- TE = echo time
- TR = repetition time

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