Comparison of direct flow simulation in a random packed bed of Raschig rings with a macroscale momentum-sink approach

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Abstract. The purpose of the work is to investigate two numerical models of gas flow in a random packed bed of Raschig rings – one based on direct numerical simulation of flow at the level of individual particles and the other simplified approach in which the bed is treated as a homogeneous domain with prescribed pressure drop calculated from Darcy law. The latter model is usually preferred when only average flow characteristics are important in a given application and is expected to provide reasonably accurate results at the macroscopic level. The results show that when the flow enters the bed in a highly non-uniform manner (here – as a jet), the simplified model is not able to reproduce velocity field even averaged over regions of a considerable size. However, the axial average pressure profile is predicted with a good accuracy.

1. Introduction
Wide applications of random packed beds in many areas of industry (e.g. in chemical engineering as catalytic reactors [1, 2]) sparked large interest in experimental and numerical investigations of flows in such complex structures. However, direct numerical simulations (PRDNS - Particle Resolved Direct Numerical Simulation) of flows in packed beds are very demanding from the computational point of view. They require accurate microscale representation of the bed geometry and high grid resolution for reliable solution of flow between the particles, so usually calculations of this type are limited to beds of relatively small size or small parts of larger structures [3, 4]. For many applications such a detailed study of flow is not necessary and macroscale approach in which only averaged flow characteristics are of interest has become quite popular. In this approach the packed bed is treated, like other porous media, as a homogeneous region of the computational space where the flow equations are supplemented with additional sink terms related to the momentum loss in the inter-particle space (see for instance porous medium model in ANSYS Fluent software [5]):

\[ S_i = - \left( \sum_{j=1}^{3} D_{ij} \mu U_j + \sum_{j=1}^{3} C_{ij} \frac{1}{2} \rho |\mathbf{U}| U_j \right) \]  

(1)

where \( S_i \) represents \( i \)-th component of the sink term, \( U_j \) – \( j \)-th component of flow velocity \( \mathbf{U} \), \( \mu \) – dynamic viscosity, \( \rho \) – density, and \( D_{i,j} \), \( C_{i,j} \) are tensors describing potentially anisotropic...
characteristics of the porous medium. Second sum on the right hand side introduces inertial effects for large velocities and can be neglected in low velocity regime. When the porous medium can be assumed to be isotropic, formula (1) reduces to:

\[ S_i = - \left( \frac{\mu}{\alpha} U_i + C_2 \frac{1}{2} \rho |U| U_i \right), \]  

(2)

where \( \alpha \) is the permeability of the medium and \( C_2 \) – inertial constant. The first term corresponds to the Darcy law and the formula (2) can be treated as its generalisation (Darcy-Forchheimer law [6]).

Models of this type are used in a considerable amount of literature works – see for example [7, 8, 9] or more complicated versions taking into account variations of local porosity and empirical formulas for pressure drop (e.g. Ergun correlation) [10, 11].

The aim of the present study is to verify how well this simplified momentum-sink approach (here abbreviated as “MSA”) reflects the real averaged characteristics of air flow in a random packed bed of Raschig rings. The PRDNS model is based on the methodology previously developed by the author in [4, 12]. The work concentrates on the laminar regime in which viscous stresses are the main component of momentum loss.

2. Methods

2.1. Flow configuration

The considered flow configuration is shown in Fig. 1a. The particles, rings of equal height and diameter, \( H_p = D_p = 0.025 \) m, with inner diameter \( D_i = 0.02 \) m, are randomly packed using the algorithm from [4] in a cylindrical container of diameter \( D_c = 0.25 \) m. Then, a section of the generated bed of height \( L = 0.24 \) m, sufficiently far from the bottom of bed to eliminate the ”bottom effect” [13], is placed in a cylindrical column of height \( H_c = 0.36 \) m and also of diameter \( D_c \), leaving two empty buffer zones of heights \( L_{b,in} = 0.09 \) m (above the bed) and \( L_{b,out} = 0.03 \) m (below the bed). The air flow enters the domain with a uniform profile at the top through a circular orifice of diameter \( D_{in} \) which equals: a) \( D_c \), uniform flow case; b) \( D_p \), jet case. The air properties are taken as \( \rho = 1.15 \) kg/m\(^3\), \( \mu = 1.85 \times 10^{-5} \) Pa·s.

On all solid walls (column, particle surface) no-slip boundary condition is imposed, on outflow plane the pressure is assumed to be 0. Flow characteristics are examined on three control planes: \( P1 \) slightly above the bed inlet (\( y = 0.3 \) m), \( P2 \) just below the bed inlet (\( y = 0.2 \) m) and \( P3 \) near the bed outlet (\( y = 0.1 \) m).

2.2. PRDNS model

The model for direct flow simulation consists of two components: bed structure generator [4, 12] and flow solver based on Immersed Boundary Method (IBM) [14, 15]. The random packing of rings is obtained in a separate simulation by sequential deposition of particles until mechanical equilibrium is attained. Although the mechanics of the process is substantially simplified, the final structure correctly reproduces not only porosity distribution but also distribution of particles’ orientation [12, 13]. The flow solver employs structured (Cartesian), staggered computational grid and projection method for solution of the flow equations – Navier-Stokes equations for incompressible fluid of constant density and viscosity – given as follows:

\[ \rho \frac{\partial U}{\partial t} + \rho U \cdot \nabla U = -\nabla p + \mu \nabla^2 U , \quad \nabla \cdot U = 0 \]  

(3)

where \( U = (U_1, U_2, U_3) = (u, v, w) \) – flow velocity and \( p \) – pressure. The complex geometry of the bed influences the flow in the prediction and the correction step of the projection method [16, 17] by damping the flow velocity near the solid boundaries. The details of the method are
Figure 1. Flow configuration (a) and sample results of PRDNS calculations for flow velocity magnitude in three cross-sections (jet case) (b).

presented in [4] and sample results for the considered flow configuration (jet case) are shown in Fig. 1b.

The grid resolution in all cases was 160 × 192 × 160 cells for the domain of size 0.25 m × 0.36 m × 0.25 m (the second dimension along the column’s axis - y), a box in which the physical domain (column) is inscribed. As shown in [4], the selected resolution should be sufficient in the analysed flow regime.

2.3. Momentum-sink model (MSA)
The momentum-sink model differs from the PRNDS model by the treatment of the bed region. Here it assumed that this is an empty space but with additional term $S$ on the right hand side of the Navier-Stokes equation (3). As it was verified that Darcy law describes with a good accuracy the relation between flow velocity and pressure gradient in the considered range of velocities and, moreover, the random packed bed of rings (except for near-wall regions) is isotropic at the macroscale [13], the momentum-sink term was taken as: $S_i = -\beta U_i$, with $\beta = \mu/\alpha$. Constant $\beta$ has been found using uniform flow test case ($D_{in} = D_c$) with different values of inlet velocity $v_g$. The steady state average pressure gradient along the bed axis turns out to be nearly constant in this case (see [4] for comparison) and the proportionality constant between $v_g$ and $dp/dy$ equals 10.8 [Pa·s/m²] (see Fig. 2a).

The uniform flow case is a perfect configuration from the point of view of momentum-sink model, as the averaged characteristics from the PRDNS simulation almost exactly correspond to the ones obtained with this simplified approach. The purpose of the next section is to examine the jet case i.e. the flow configuration in which the air enters the bed in a highly non-uniform manner.

3. Results
In the main part of this work, simulation has been performed of a jet injected with velocity 0.2 m/s along the column’s axis through an orifice of diameter $D_{in} = D_p$ and impinging on the bed.
Figure 2. Relationship between the pressure gradient in the bed and the inlet velocity for uniform flow case (a); the axial average pressure profile for the jet case (b).

\((Re = 311)\). This test case gave an opportunity to examine developing non-uniform flow in the empty space above the bed and the bed itself. When the steady state was reached, the results obtained with the momentum-sink model could be compared with the spatially averaged results of direct simulations in the real geometry of the packing. The average value of flow property (velocity component or pressure) has been calculated with the PRDNS model at a given point \(P\) by finding arithmetic mean of this property in the sphere centred at \(P\) and with radius \(R_{av}\). Of course, the averaging is limited to the bed region. Three values of averaging radius have been examined \(R_{av} = 10h, 20h, 30h\), where \(h\) – size of the computational cell. These values correspond to \(R_{av} = 0.625D_p, 1.25D_p, 1.875D_p\), respectively.

The axial average pressure profile has been found by averaging over domain cross-sections normal to the column axis. As it can be seen in Fig. 2b, even for the jet this pressure profile coincides with the solution from the PRDNS model with the differences not larger than a few percent.

Unfortunately, one cannot say the same about flow velocity components. In Fig. 3 three contour plots for streamwise component \(v (U_2)\) are shown at the axial cross-section of the column for the PRDNS model (a), averaged solution from the PRDNS model (b) and MSA model (c). For convenience of visual comparison, the colour variations represent the range of negative values of \(v\) (mean flow direction) not larger than 10 mm/s in magnitude. What immediately leaps to the eye is the different structure of the flow above the bed and the fact that the flow inside the bed found with the MSA model becomes essentially uniform after quite a short distance (\(\approx 0.5L\)).

Fig. 4 gives an opportunity for more quantitative comparisons of the results. Spanwise components \(u, w\) are taken from respective control planes \((P1, P2, P3)\) and line segments described by \(z = 0\), variable \(x (u\ component)\) or \(x = 0\), variable \(x (w\ component)\). Due to symmetry of the domain and the inflow conditions, in the case of MSA model the flow is almost axisymmetric so only one component is shown \((u)\). Of course, in the PRDNS model the geometry of the bed is far from being symmetrical at the particle level (microscale) and significant differences occur between \(u\) and \(w\) components, even after averaging over a broad region.

The influence of averaging is shown in Fig. 5. It can be noticed that increasing of \(R_{av}\) leads to smoothing of irregularities of velocity components (as could be expected) but, at the same time, the non-uniformity of the flow also tends to even out and the very object of the examination dissolves into uniform field (see particularly the evolution of \(u\)). Thus, the value of \(R_{av}\) cannot
Figure 3. Streamwise velocity component $v$: the flow in the real geometry of the bed (a), spatially averaged PRDNS solution ($R_{av} = 30h$) (b) and the solution based on the momentum-sink approach (c).

be too large and, as a compromise, $R_{av} = 20h$ was taken for the remaining graphs.

As can be seen from the other graphs in Fig. 4, only streamwise component in plane $P_1$ is reproduced well by the MSA model, except for the neighbourhood of the jet entrance into the bed where distinct backflow is wrongly predicted. The difference between magnitudes of velocity components is significant, in terms of relative error particularly large in $P_3$ plane where the MSA model predicts considerable uniformisation of the flow, as already noted in Fig. 3.

As for the distribution of average pressure across the column diameter (Fig. 6), in contrast to the axial profile, the MSA model greatly underestimates the maximum near the bed inlet ($P_1$) but, on the other hand, reproduces the pressure distribution near the bed outlet ($P_3$) with the relative error of order of only 20%.

4. Conclusions

Although the MSA model allows for significant computational advantage comparing to the PRDNS model one should bare in mind the limitations of the simplified approach. At least in the considered test case of an air jet developing in the random packing of Raschig rings, the MSA model is not able to predict the distribution of flow velocity components when averaging is performed at the scales comparable with the diameter of the container. The uniformisation of the flow in the exact model occurs much further beyond the bed inlet and even after distance comparable with the container diameter the streamwise component is dominant near the column axis. On the other hand, the axial average pressure profile and pressure distribution at large distance from the bed inlet are predicted by the MSA model with an accuracy of a few percent.

The general observation is that the proper reproduction of flow velocity inside a random packed bed at the macroscale requires much more sophisticated models than a momentum-sink term representing the Darcy law (even in the low velocity regime).

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Figure 4. Profiles of streamwise (v) and spanwise velocity components (u,w) in three control planes.

Figure 5. The influence of averaging radius $R_{av}$ on average velocity profiles
Figure 6. Average pressure profiles in planes $P_1$ and $P_3$.

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