CFD modelling of gas flow through a fixed bed of Raschig rings

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Abstract. In this work, direct numerical simulation of incompressible gas flow through a complex geometrical structure of Raschig rings is performed. The bed structure is obtained in a separate simulation in which Raschig rings are added one by one and fall freely into a cylindrical container until mechanical equilibrium is reached. The gas is injected at the top of the container, flows through a packed layer of randomly oriented rings, then leaves the container at the bottom. The flow equations are solved with the use of classical second order solver and projection method for structured regular grid and the complexity of domain geometry is handled by a variant of immersed boundary technique. The model allows to study the characteristics of the flow within the bed, pressure distribution in particular, and can be applied to development and validation of simplified approaches. The simulations are performed for various grid resolutions and the results show good convergence to grid independent solution, especially for lower gas velocities. The obtained dependence of total pressure drop on the inlet velocity is in reasonable agreement with the literature data but the demand for grid resolution significantly increases with the gas velocity.

1. Introduction
A fluid flow through a porous bed, because of highly complex domain geometry, is usually modeled in a simplified fashion using averaged flow equations [1,6]. Such an approach does not require generation of equally complex computational grids and also allows for simulation of full-scale systems taking into account many phenomena essential from the point of view of a given process.

However, for simplified modeling it is necessary to deliver some information about porosity of the bed (or the distribution of porosity when it is not homogeneous), active surface of the bed elements and the influence of the microstructure of the bed on the flow characteristics in a larger scale. Such data can be obtained only in experiments [2,3] or in advanced CFD simulations when the physics of fluid flow in complex geometry is properly captured [4,5].

In a recent publication [7] a method has been presented of numerical generation of a fixed bed structure consisting of cylindrical elements or - after a minor modification – Raschig rings. The idea of the method is to simulate the filling process of a cylindrical container with bed elements added one-by-one, moving due to gravity and reaction forces from the remaining bed elements until eventually mechanical equilibrium is reached. Then a given element is included in the bed structure and remains at rest to the end of the simulation. Structures generated in this way can be examined with respect to porosity distribution to obtain necessary input for averaged flow equations or used directly in CFD simulations as the geometry of the computational domain.
This work is devoted to direct numerical simulation of gas flow through a fixed bed, a cylindrical container filled with Raschig rings, of numerically generated realistic structure. Examination of the flow at the microscopic level can be very useful from the point of view of construction of models focused on larger scales as well as validation of models already formulated on the basis of experimental research. One of the main results obtained here – pressure drop in the bed – is of importance for practitioners designing systems with fixed beds e.g. absorbers.

The plan of the paper is as follows. In Section 2 the flow solver is shortly described. Section 3 presents the results of pressure drop calculations together with grid convergence studies and comparison with reference experimental data. Section 4 closes the paper with summary.

2. Flow solver
In this section, solution of Navier-Stokes equations for incompressible flow is described, together with a variant of Immersed Boundary Method used for handling of complex domain geometry.

2.1. Solution of flow equations (simple geometry)
The flow solver Drifter, in-house code developed at Institute of Thermal Machinery, is a classical second order finite volume code based on staggered MAC grid and projection method [8]. As it was designed for simulation of flow in simple academic geometries, the complex bed geometry is handled by a variant of immersed boundary method [10].

The full computational domain is rectangular box circumscribed on the cylindrical container (see figure 1). Physical dimensions of the box in x and z direction coincide with the diameter of the container and the dimension in y direction depends on the height of the considered bed (possibly including empty buffer zones above and beneath the bed). The number of grid nodes in each direction can be set independently as \( N_x, N_y, N_z \).

Assuming that velocity \( \mathbf{u} \) of incompressible flow is expressed as \( \mathbf{u} = [u, v, w] \), Navier-Stokes equation can be written as [8,9]:

\[
\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \nabla \cdot \mu \left( \nabla \mathbf{u} + \nabla \mathbf{u}^T \right) - \rho g, \quad \nabla \cdot \mathbf{u} = 0 \tag{1}
\]

where \( \rho \) - density, \( p \) - pressure, \( \mu \) - dynamic viscosity, \( g \) - gravitational acceleration.

Flow equations (1) are solved with projection method in three stages. In the first, the pressure term is omitted – equation (1) takes the form of advection-diffusion equation with a source term – and provisional velocity \( \mathbf{u}^* \) is found. In the second stage, Poisson equation is solved for pressure with the right hand side of the equation depending on the divergence of the provisional velocity (this is the most time consuming part of the whole procedure). In the third stage, when the pressure is known, the provisional velocity is corrected and the flow velocity in the next time step is obtained.

The solution is advanced in time with second order Runge-Kutta scheme. The advection term is treated with second order upwind scheme and the diffusion term with the central second order finite difference formula. The Poisson equation is discretised with second order central finite difference in space and the resulting set of equations is solved with preconditioned conjugate gradient method (IPCG). The preconditioner is based on incomplete Cholesky decomposition.

2.2. Handling complex geometry on regular grid
In the literature, there are examples of flow simulations in complex realistic bed structure [4,5]. The methods used, however, require generation of highly complex computational grids fitted to the considered structure (usually simplified e.g. by using spherical bed elements). The approach taken in this work is completely different and enables simulation of flow through the bed on regular structured grid.
Immersed boundary method (IBM) was originally formulated by Peskin [10] for simulation of blood flow in heart (dynamically changing geometry) using structured grid. The main concept of the method has been the modelling of “immersed” boundaries by proper source terms in flow equations. In the following years, a large number of variants of the method has been developed. It can be shown [9] that in the case of stationary boundaries (fixed geometry) and no-slip boundary condition, additional source terms are not necessary. The approximation of the appropriate boundary condition and the damping of flow velocity on the immersed boundaries can be realized by modification of provisional velocity in the first stage of projection method:

\[
\mathbf{u}^* = \mathbf{u}_0^* b(\varphi)
\]

where \( \mathbf{u}_0^* \) - provisional velocity calculated as described in 2.1., \( \varphi \) - signed distance of a given point from the immersed boundary. The distance can be easily calculated for a single ring (or container wall) and then the minimum value is taken over all the bed elements. For the points inside the ring’s shell the distance is negative (hence the term: “signed” distance). The damping function \( b \) should be equal 1 far from immersed boundaries (no damping) and equal 0 inside the ring’s shell (full damping). In order to avoid numerical difficulties with discontinuous function, a transition zone is introduced in the definition of function \( b \):

\[
b(\varphi) = \begin{cases} 
1 & \text{for } \varphi > \Delta h \\
1 + \frac{1}{2} \sin \left( \frac{\pi (\varphi - \Delta h)}{\sigma h} \right) & \text{for } -\Delta h < \varphi < \Delta h \\
0 & \text{for } \varphi < -\Delta h
\end{cases}
\]
where \( h \) is the grid step, \( \Delta, \sigma \) - parameters of the damping function describing the shift and the smoothing width. The degree of smoothing should be large enough to filter out the irregularities of provisional velocity near the immersed boundary. However, the smoothing cannot be too large as it widens the area of influence of the boundary on the grid points in the interior of the domain.

The parameters of the damping function have been selected in a test case of a laminar flow through a circular channel (without rings), for which the analytical solution is known and the velocity profile together with the pressure drop may be used as reference data for simulation results.

The simulations were performed for three computational grids differing by number of nodes on the channel cross-section (5×5, 10×10, 20×20 grid points respectively) and for three values of Reynolds number (5, 250 and 1000). Parameters \((\sigma, \Delta)\) were selected to obtain the minimum error of pressure drop value for all considered cases. This resulted in \( \Delta = -0.1 \) and \( \sigma = 0.3 \).

Beside the change of the provisional velocity, similar damping is applied to corrected velocities (third stage of projection method). Sample distribution of \( b(\varphi) \) field for a bed of Raschig rings is shown in figure 2. The distance \( \varphi \) is understood not only as the distance from the nearest ring but also from the container wall.

To summarise, a single time step of projection method is realised in the following substeps:

a. Calculation of provisional velocity \( u^*_0 \), then modified with the damping function \( u^* = u^*_0 b(\varphi) \).

b. Solution of pressure equation: \( \nabla^2 p = \rho \nabla \cdot u^*/\Delta t \), where \( \Delta t \) - time step.

c. Correction of provisional velocity: \( u^{**} = u^* - \nabla p \Delta t / \rho \) and the final damping \( u^{n+1} = u^{**} b(\varphi) \).

3. Simulation of gas flow through the fixed bed

This section presents sample results of simulation of gas flow through a fixed bed of Raschig rings. The gas is injected at the top of the domain with uniform velocity profile. In the considered range of inlet velocity, the flow within the bed remains in the laminar regime. As the flow velocity is damped
on the container wall and on the rings’ boundaries, this represents no-slip boundary condition. At the outlet (bottom of the domain) zero gradient boundary condition is imposed on the velocity. In the case of pressure Neumann boundary condition is used for the inlet plane and side walls, and Dirichlet boundary condition at the outlet. The computational domain covers the whole container and two empty buffer zones above and below the bed.

Looking at the iso-surface of vorticity (figure 3a), we can see complex structure of the flow inside the bed. Although some longer vortex tubes may be distinguished, the flow is generally irregular which is not surprising bearing in mind the random packing of rings. The distribution of pressure (figure 3b) reveals distinct pressure gradient and local variations of the pressure due to local changes in bed porosity.

Figure 3. Gas flow through the bed: a) iso-surface of vorticity, b) pressure distribution in cross-sections of the domain.

A good quantitative test is an examination of pressure gradient dependence on the gas velocity \( v_g \) at the inlet. In the literature, empirical formulas can be found for pressured drop in the beds consisting of various elements and for different flow conditions. For instance, Billet proposes [11]:

\[
\frac{\Delta p}{H} = \xi \left( \frac{64}{\text{Re}_v} + \frac{1.8}{\text{Re}_v^{0.08}} \right),
\]

\[
\text{Re}_v = \frac{v_g d_p \rho_v}{(1-\varepsilon) \eta_v}, \quad d_p = \frac{1-\varepsilon}{a}, \quad \frac{1}{f_s} = 1 + \frac{4}{ad_s},
\]

where: \( \varepsilon \) - bed porosity, \( \rho_v \) - gas density, \( a \) - geometric surface are of packing per unit volume,

\[
\xi_0 = C_p \left( \frac{64}{\text{Re}_v} + \frac{1.8}{\text{Re}_v^{0.08}} \right)
\]

where: \( \eta_v \) - gas viscosity, \( C_p = 1.329 \) for Raschig rings, \( d_s \) - container diameter.
In [12] Maćkowiak suggests another formula (based on a wide range of empirical data):

\[ \frac{\Delta p}{H} = \psi_0 (1 - \phi_p) \frac{1 - \rho_v \varepsilon^2}{\varepsilon^3 d_p K} \]  

(7)

where: \( \phi_p \) - proportion of perforated surface area of the bed element (equal 0 for Raschig rings) and \( K \) is a coefficient taking into account the influence of the finite diameter of the container (analogous to \( f_s \) in Billet formula):

\[ \frac{1}{K} = 1 + \frac{2}{3} \frac{d_p}{d_s} \]  

(8)

and

\[ \psi_0 = \frac{725.6}{\text{Re}_v} + 3.203 \]  

(9)

Figure 4. Calculated pressure gradient as the function of gas velocity and grid density. Solid and dashed line represent the values calculated with empirical formulas.

The simulation results for a bed consisting of 1056 rings \((a = 193.6)\) is shown in figure 4. The curves represent the values calculated with empirical formulas of Billet and Maćkowiak. It can be seen that in the considered range of gas velocities the difference between them is not large. The simulations were performed for computational grids of various densities to examine the influence of the grid on the results and the convergence of the solution with sufficient level of accuracy. The cases are denoted as g080, g120, g160, g200 and g240, respectively, for grids of \(80 \times 80 \times 96\), \(120 \times 120 \times 144\), \(160 \times 160 \times 192\), \(200 \times 200 \times 240\), \(240 \times 240 \times 288\) nodes. The transition from one case to the next one resulted in approximately doubling of the computational time required to attain steady state flow and final value of pressure drop.

The obtained results show distinct sensitivity to the number of grid nodes for larger values of gas velocity. This may be related to the change of flow character (regime), separation of boundary layers and no explicit model in the solver to take into account such effects. However, for values of gas velocity lower than 0.15 m/s the convergence of the solution is quite satisfactory and for the finest
mesh (g240) the correction of pressure gradient is not larger than 3%. Comparing the simulation results with empirical formulas one should bear in mind considerable level of uncertainty of the latter ones (reaching even 20%), as typically they are derived as the correlation of a wide range of bed and flow parameters.

4. Summary
In this work, simulation gas flow through a porous bed has been performed by directly solving flow equations in the realistic geometry. Such an approach allows for capturing the physics of the process and construction or verification of various models designed for larger scales. The obtained values of pressure drop within a bed show good convergence with increasing grid density and do not deviate much from empirical formulas derived for the beds of industrial scale.

In future work, the model will be extended with two-phase flow simulation capabilities in order to analyse the structure of liquid flow through a fixed bed which is important in some industrial applications (e.g. absorbers).

5. References

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