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CFD-based modelling of the residence time distribution in structured fixed beds

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Fixed bed reactors are well known in chemical industry. These reactors are usually modelled using a pseudo-homogeneous approach and experimentally determined correlations. This simplified description does not permit a detailed analysis of the liquid flow between the particles, where local phenomena are particularly important, significantly influencing the overall reactor performance.
In this work, complex local flow field patterns in fixed bed reactors are studied. Two different regular arrangements of spheres are investigated using the commercial computational fluid dynamics code CFX by ANSYS Inc. To validate the simulation results, Ergun and Carman pressure drop correlations are used. Numerical simulations are in a good agreement with both correlations. Furthermore, the residence time distribution is estimated using two different methods.

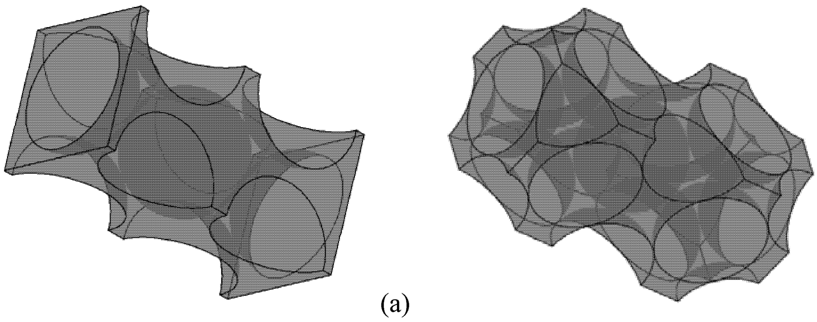
1. Introduction

Fixed bed reactors are 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, fixed bed reactors will most probably be still in use in the forthcoming decades, mainly because of their low cost (Calis et al., 2001).
Hydrodynamic and transport properties of packed beds can be studied using two different numerical approaches. In the first one, fixed beds are treated as a pseudo-homogeneous media, by application of modified Navier-Stokes equations and the continuity equation. In this set of equations, an additional term is used describing the porosity distribution in order to take into account the packing geometry. The porosity distribution most commonly is based on empirical correlations (Freund et al, 2003).
In the second approach, the packed bed is simulated with due account of the actual packing 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 spheres, two different methods are used. The first one is the lattice Boltzman method (LBM). Using the LBM, Freund et al. (2003) calculated the local velocity and the pressure drop in random arrangements of spheres in rectangular containers. Simulation results are in a good agreement with experimental data. The dispersion coefficient in packed beds was investigated by Manz et al (1999) and Zeiser et al. (2001).
In the second method, the Navier-Stokes equations are resolved for the void between the spheres. In the work of Calis et al. (2001), the local velocity field in both regular and irregular configurations of spheres is studied in rectangular containers for channel diameter/particle diameter ratio up to four. Furthermore, Nijemeisland and Dixon

(2004) investigated the relationship between the local flow field and the local wall heat flux in a packed bed of spheres. Kloeker et al. (2005) studied the mass transfer for different Reynold numbers in arranged spherical geometries. Similar arrangments are used in the present work.
Our objective is to study the local velocity field in a fixed bed of spheres using computational fluid dynamics (CFD). Numerical results on pressure drop for different Reynolds numbers are compared with correlations based on experiments. For the determination of the residence time distribution (RTD), two different methods are employed and compared.

2. Studied geometries

In this work, two different arrangements of spheres with diameter equal to 0.001 m and different porosities are considered. These arrangements follow the arrangements of atoms in ideal crystals, namely the body-centered cubic (bcc) and the face-centered cubic (fcc) arrangements. The void fraction of the bcc and fcc configuration are 0.32 and 0.26, respectively. The constructed geometries are depicted in Fig. 1.



(a) (b)

Figure 1 Body-centered cubic (a) and face-centered cubic (b) spherical arrangements (Kloeker et al., 2005).

Due to the complex geometry, an unstructured tetrahedral grid is used for an appropriate discretisation of the computational domain. Special attention is paid to resolve accurately the boundary conditions near the particle surface, where prismatic elements are used. To obtain grid independent results, more than one million tetrahedral and prismatic elements are necessary.
To simulate the fully developed flow neglecting inlet and wall effects, periodic boundary conditions are imposed at the inlet and outlet of the domain, along the main flow direction. The use of periodic boundary conditions reduces the domain length resulting to a substantial reduction of the required computational power and time. Simulations are performed using a commercial CFD software code CFX by ANSYS Inc.

3. Hydrodynamics

As a first step, the hydrodynamics of the constructed geometries is analysed. For all simulations, water at 20 °C is used as a fluid medium. To validate the simulation results, pressure drop correlation are used, namely the Ergun and Carman correlations (Eisfeld and Schnitzlein, 2001). Both correlations are applied in a non-dimensional form, using the dimensionless pressure drop defined by

$$\psi = \frac{\Delta P}{L}\frac{d_p}{\rho\, U_0^2} \tag{1}$$

where ΔP is pressure drop, L is length of the packing, d_p is particle diameter, ρ is density and U_o is superficial velocity. The particle Reynolds number is given by

$$Re_p = \frac{d_p\, \rho\, U_0}{\mu} \tag{2}$$

where μ is viscosity. Ergun correlation as a function of the dimensionless pressure drop ψ is expressed as

$$\psi = \frac{A}{Re_p}\frac{(1-\varepsilon)^2}{\varepsilon^3} + B\frac{(1-\varepsilon)}{\varepsilon^3} \tag{3}$$

where ε is void fraction of the packing. The constant values for Ergun correlations are A=150 and B=1.75. Carman correlation is defined as

$$\psi = \frac{6^2}{Re_p}k\frac{(1-\varepsilon)^2}{\varepsilon^3} \tag{4}$$

with k=5 for spherical particles in the laminar flow regime (Eisfeld and Schnitzlein, 2001).

In Fig. 2, simulation results for different Reynolds numbers are compared with the results obtained by Eq. (3) and Eq. (4). For the *distinguishing streamline* flow region ($Re_p < 10$), numerical results agree well with both correlations. For higher particle Reynolds numbers at the *transitional* flow regime ($10 \le Re_p \le 300$), numerical results

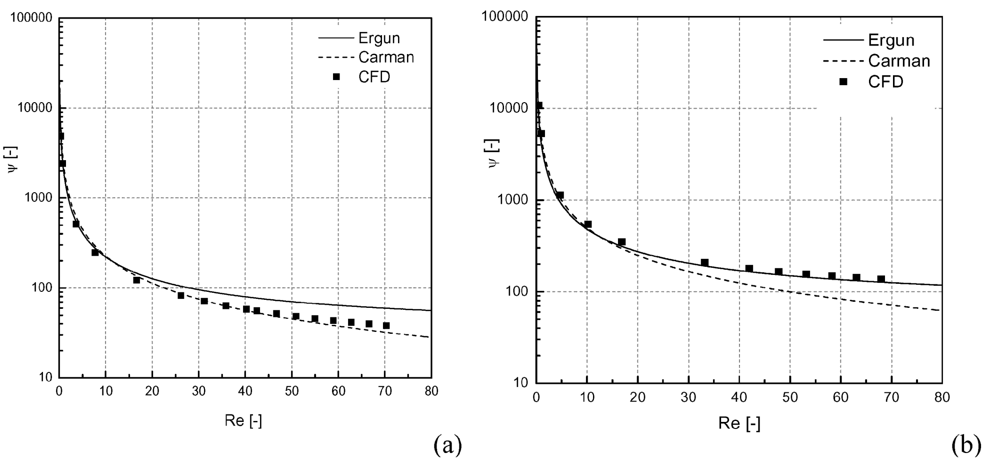


Figure 2 Comparison of the pressure drop for different Reynolds numbers for the bcc (a) and the fcc (b) spherical configuration.

of the bcc arrangement agree better with Carman correlation, while results of the fcc arrangement with Ergun correlation. In both cases, pressure drop values predicted by the CFD model and by the both correlations are in the same range.

In Fig. 3, the velocity distribution is shown for a particle Reynolds number of 5. In the bcc arrangement, higher local velocities can be observed in comparison to the fcc arrangement. This is because of the higher local void fraction of the bcc arrangement. Additionally, in the bcc configuration, stagnant zones can be observed at the front and rear of each particle. For the fcc configuration, they are less extensive. These zones are not desirable in chemical processes since, without convective flow, mass and heat transfer is slow.

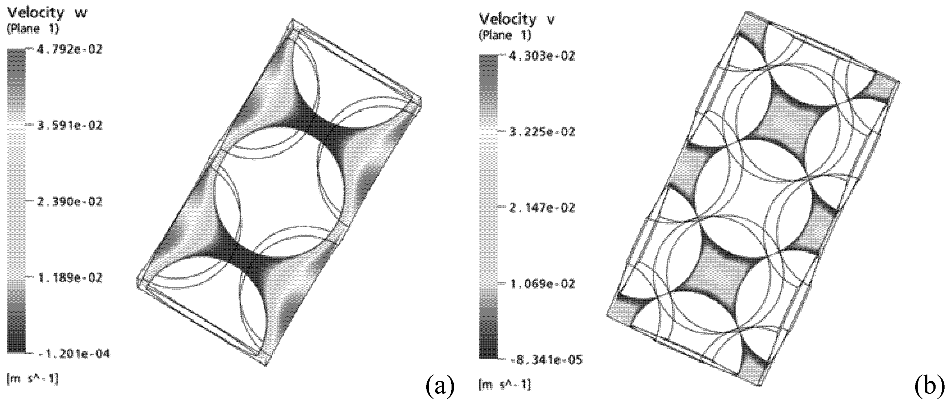


Figure 3 Velocity distribution along the main flow direction for particle Reynold number equal to 5 for the bcc (a) and the fcc (b) arrangement.

4. Residence time distribution

Flow through a fixed bed reactor usually deviates from ideal plug flow. Liquid channelling effect or stagnant liquid zones are undesirable phenomena for chemical processes. Therefore, it is important to analyse and better understand the reasons of the liquid maldistribution in fixed bed reactors, and CFD models serve as useful tool towards this direction.

For the determination of the residence time distribution (RTD) in fixed bed reactors, two different approaches are employed and compared here, namely *the tracer method* and the *post-processing method* (Levenspiel, 1999).

The first one imitates the experimental approach for the determination of the RTD. A non-diffusive tracer is injected into the computational domain using a Dirac function. The change of the tracer concentration, both in time and space, provides the RTD. The average (over the reactor cross-section) residence time can be determined as follows

$$\overline{\tau} = \frac{\int_0^\infty t\,\overline{C}(z,t)\,dt}{\int_0^\infty \overline{C}(z,t)\,dt} \qquad (5)$$

where $\overline{C}$ is averaged tracer concentration over the cross-section at the longitudinal coordinate z and t is time. In the post-processing method, the RTD can be evaluated directly, once the velocity field is known. The local residence time can then be obtained from the solution of the following equation (Ghirelli and Leckner, 2004):

$$u\,\nabla\,\tau = 1 \qquad (6)$$

where u is local velocity. The RTD calculated with the post-processing method is depicted in Fig. 4. For the bcc configuration, regions with high residence time are observed at the rear of the particles.

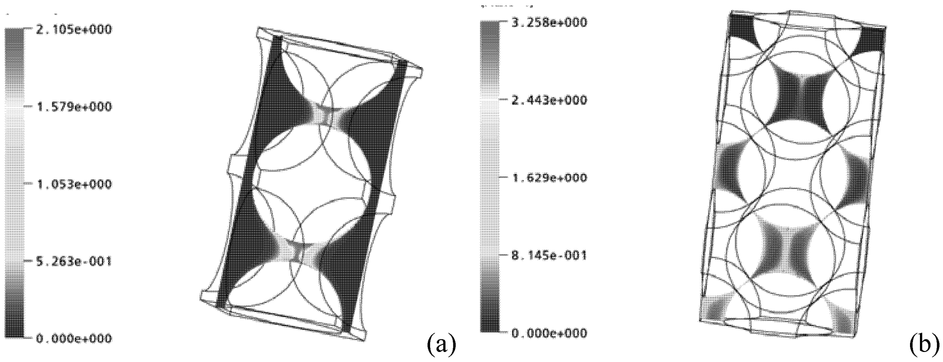


Figure 4 RTD in seconds using the direct calculation of the age distribution for the bcc (a) and the fcc (b) arrangement.

A comparison between these two methods for different heights z of the packing is presented in Fig. 5. Both methods give similar results. The main advantage of the post-

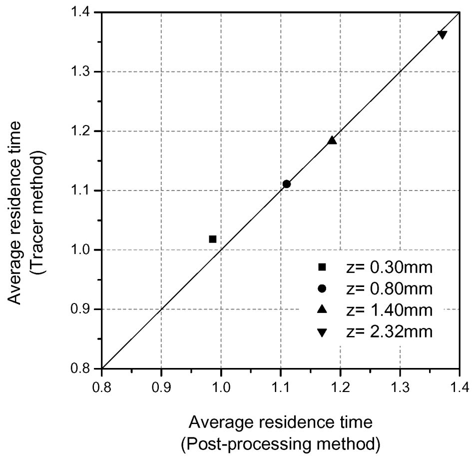


Figure 5 Comparison of average residence times obtained by the tracer and by the post-processing method at different packing heights z.

processing method is that it requires less computational time and power compared to the tracer method.

5. Conclusions

In this work, the local hydrodynamics in regular beds of spheres is studied. Two different bed configurations with different porosities are constructed. In all simulations, wall and inlet boundary are neglected.
For the validation of the simulation results, two pressure drop correlations are used, namely the Ergun and the Carman correlation. Numerical results are in a good agreement with both correlations.
For the bcc configuration, stagnant zones can be observed at the front and rear of each particle. These zones are less extensive for the fcc configuration. Generally, in industrial applications, such zones are not desirable, since they result in slow mass and heat transport.
Two different methods are used for the estimation of the RTD. The tracer method imitates the experimental procedure using a non-diffusive tracer, whereas the post-processing method directly calculates the RTD from the local velocity field. Both methods give similar results. The post-processing method is preferable, since it requires less computational power and time compared to the tracer method.
In the future, the inlet effect and the influence of the wall on the fluid dynamics will be studied for both regular and irregular packed beds. In this way, a more realistic representation of the actual configuration in fixed bed reactors can be achived.

6. Acknowledgement

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