

A numerical study on the residence time distribution in low and moderate tube/particle diameter ratio fixed bed reactor

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Fixed bed reactors are extensively used in chemical industry. Knowledge on local velocity distribution is particularly important for the understanding of the overall reactor performance in terms of pressure drop, residence time distribution, heat and mass transfer coefficients.

In this work, such velocity fields are studied taking into account the effect of the confining walls. Irregular particle arrangements are investigated using the commercial computational fluid dynamics code CFX 11.0 by ANSYS Inc. The arrangement geometry is built based on a modified ballistic deposition method. To validate the simulation results, pressure drop correlations from literature are used. Numerical simulations are in a good agreement with correlations that take into account the confining wall effect. Furthermore, the residence time distribution is studied using two different methods.

1. Introduction

Fixed bed reactors have been widely used in numerous industrial applications for more than 70 years. They find application 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).

The accurate estimation of the pressure drop, residence time distribution (RTD), mass and heat transfer coefficients is of crucial importance for the optimal design and operation of fixed bed reactors. In this work, we will focus on the first two parameters. A review on the influence of the confining walls on the pressure drop in packed beds was published by Einfeld and Schnitzlein (2001), whereas experimental data mainly found in the literature were compared with a number of correlations. Einfeld and Schnitzlein (2001) found that the Reichelt's approach is the most promising for the pressure drop prediction, since it shows the smallest deviation from the experimental data for a wide range of Reynolds numbers ($0.01 \leq Re_p \leq 17635$) and different fixed bed configurations (tube/particle diameter ratios $1.624 \leq \lambda \leq 250$ and average bed porosity $0.330 \leq \varepsilon \leq 0.882$).

Experimental studies on RTD in large tube/particle diameter ratio fixed bed reactors have been extensively carried out (e.g., Froment and Bischoff, 1979). However, for low and moderate tube/particle diameter ratios, even though they are applied in several industrial processes, especially in the case of highly exothermic reactions, only few studies can be found in the literature (e.g., Tang et al., 2004). For low and moderate tube/particle diameter ratios, the existence of the walls plays an important role in their overall performance. Large radial porosity variations are expected with higher porosities near the wall leading to undesirable channelling effects.

The analysis of the local velocity field in a fixed bed using computational fluid dynamics (CFD) is proven to be useful for better understanding of the phenomena occurring in the reactors. Our objective is to apply CFD methods in order to study the influence of the local velocity field on the pressure drop and RTD in different packed bed configurations. Pressure drop values obtained numerically for different flow rates are compared with experimentally determined correlations from the literature. For the evaluation of the RTD, two different methods are employed and compared.

2. Geometries studied

To build the irregular packed bed configuration of non-overlapping spherical particles, a ballistic deposition method is employed (Coehlo et al., 1997). 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 is dropped, and only the particle with the lowest final position becomes a part of the stack. In Fig. 1a, the void fraction and the number of particles are plotted against the number of “test” particles. If the number of “test” particles 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 (Kainourgiakis et al., 2002).

To govern both low and moderate ratios, we consider tube/particle diameter ratio (λ) values between 1.0 and 7.0. For this range of ratios, the wall effect on the pressure drop is significant. In Fig 1b, the generated irregular particle arrangement for $\lambda = 5.0$ is shown.

Due to the complex geometry, an unstructured tetrahedral grid is used for an appropriate discretisation of the computational domain. To avoid low quality mesh elements at the contact points between particles as well as between the particles and the confining wall, all particles are shrunk by 4% of their diameter after the initial definition of the bed. In other words, for the generation of the packing arrangement using the ballistic deposition method, particles of 1 mm diameter are used. Before the mesh generation, the diameter of each particle is reduced from 1 mm to 0.96 mm. For all the calculations, the new geometrical characteristics (average void fraction, radial porosity distribution) of the bed are estimated after this diameter reduction has been done.

During the mesh generation, special attention is paid to resolving accurately the boundary conditions near the particle surface where prismatic elements are used. In this work, we found that 5 layers of prismatic mesh elements were sufficient for the correct description of this boundary condition. To obtain grid-independent results, up to 30

million tetrahedral and prismatic elements were used; this value vary with the geometrical complexity and the considered number of particles of the fixed bed.

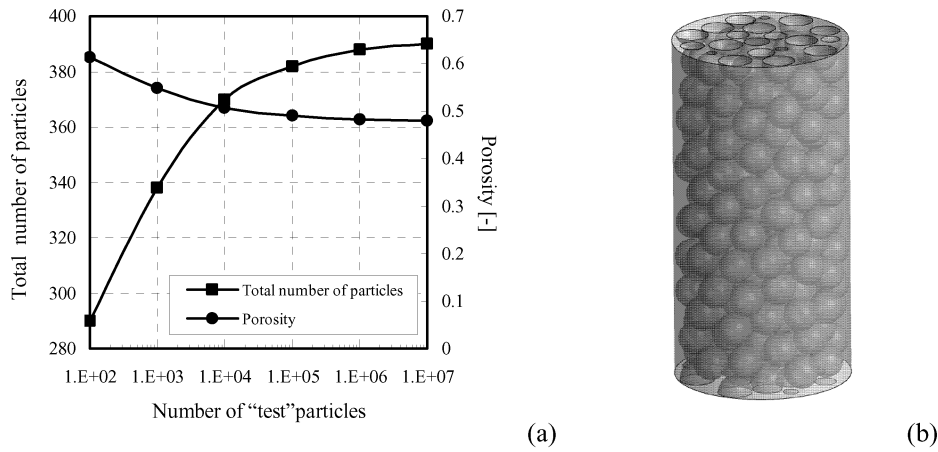


Figure 1. Total number of particles and porosity as a function of the number of "test" particles (a) and particle arrangement of the simulated irregular configuration with $\lambda = 5.0$ (b).

In order to simulate the fully developed flow, neglecting inlet effects, periodic boundary conditions are 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. At all other surfaces, the standard no-slip boundary condition is imposed.

The solution is obtained using a second-order discretisation scheme. Simulations are performed with the commercial CFD software code ANSYS CFX 11.0[®] by ANSYS Inc.

3. Hydrodynamics

For the description of the complex 3-D flow field between the particles inside a packed bed reactor, the momentum and continuity equations are used. The flow within the packed bed is considered incompressible and steady-state. The solid particles do not move and the void between them remains constant. All simulations are performed for the laminar flow regime ($Re_p < 100$), since in this regime the pressure drop changes significantly with the particle Reynolds number and hence, large variations are expected. For the simulations with $\lambda < 4.0$, air at 20 °C is used as a fluid medium; for $\lambda > 4.0$, water at 20 °C is applied. To validate the developed CFD model, the pressure drop is calculated and compared with the most common correlations, namely, by Carman, by Ergun, by Zhavoronkov et al. and by Reichelt (see Einfeld and Schnitzlein, 2001). This comparison is shown in Fig. 2. All correlations are applied in a non-dimensional form, using the dimensionless pressure drop defined by

$$\psi = \frac{\Delta P}{L} \frac{d_p}{\rho U_0^2} \quad (1)$$

where ΔP is pressure drop, L is length of the packing, d_p is particle diameter, ρ is density and U_0 is superficial velocity. The particle Reynolds number is given by

$$Re_p = \frac{d_p \rho U_0}{\mu} \quad (2)$$

where μ is viscosity.

Simulation results agree better with the correlations that take into account the wall influence. The effect of the confining wall on the pressure drop is substantial, especially or low and moderate tube/particle diameter ratio fixed bed reactors.

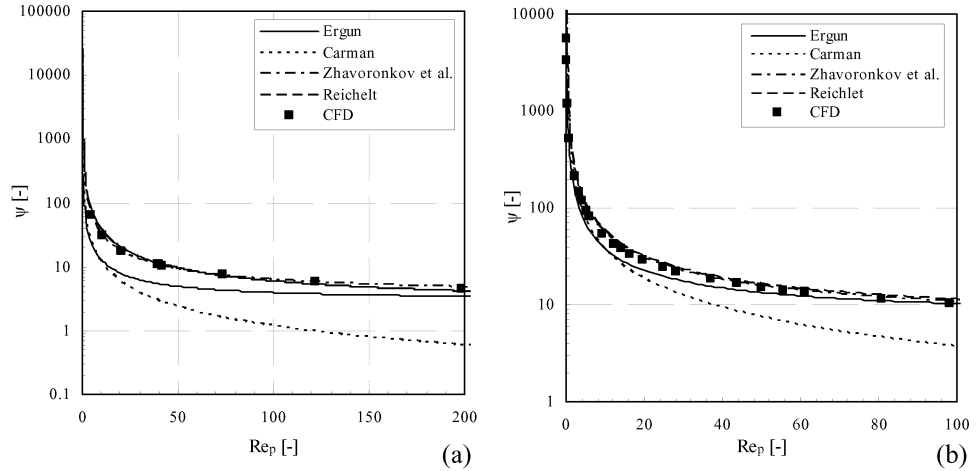


Figure 2. Dimensionless pressure drop calculated by different methods for different particle Reynolds numbers, Re_p , for $\lambda = 2.0$ (a) and for $\lambda = 5.0$ (b).

In Fig. 3a, the velocity distribution in a cross-section of the packed bed reactor is shown. Channelling is mainly observed near the wall where the 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, at the surface and behind the particles, zero velocity areas can be observed.

4. Residence time distribution

The flow through a fixed bed reactor usually deviates from the 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 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 RTD calculated with this method is depicted in Fig. 3b as a function of the dimensionless time (real simulation time divided by the mean residence time). The near-wall pick on the tracer concentration appears at lower times than the pick close to the centre. This is due to the higher velocities observed near the wall due to the channelling effect.

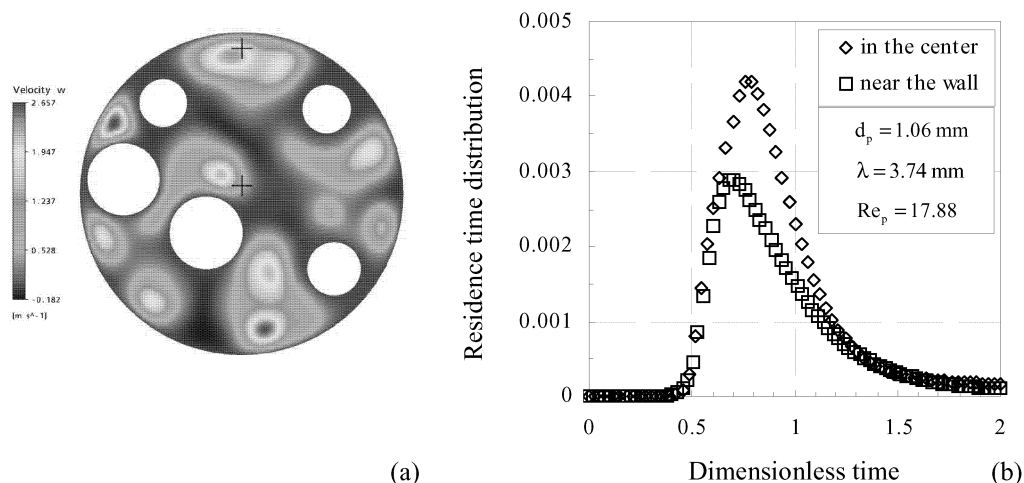


Figure 3. Velocity profile (a) and typical RTD curves for the centre and near the wall (b) for $\lambda = 3.7$. The black crosses show the positions where the RTD curves are estimated.

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):

$$u \nabla \tau = 1 \quad (3)$$

where u is local velocity and τ is local residence time. The RTD calculated with the post-processing method for different particle Reynolds numbers is depicted in Fig. 4. Both methods give similar results in terms of local averaged residence time, with deviations smaller than 5%. The main advantage of the post processing method is that it requires less computational time and power compared to the tracer method.

5. Conclusions

In this work, the local hydrodynamics, the pressure drop and the RTD in fixed bed reactors with irregular particle arrangements are studied. Different bed configurations with different tube/particle diameter ratios are considered. In all simulations, inlet effects are neglected and periodic boundary condition in the main flow direction are applied.

For the validation of the simulation results, different pressure drop correlations are used, namely correlations by Carman, by Ergun, by Zhavoronkov et al. and by Reichelt. Numerical results are in good agreement with the latter two correlations which take into

account the effect of the confining walls. For all constructed geometries, channelling is mainly observed near the wall where local void fraction is higher; it also takes place in the inner part. Zero velocities areas can be found behind the particles.

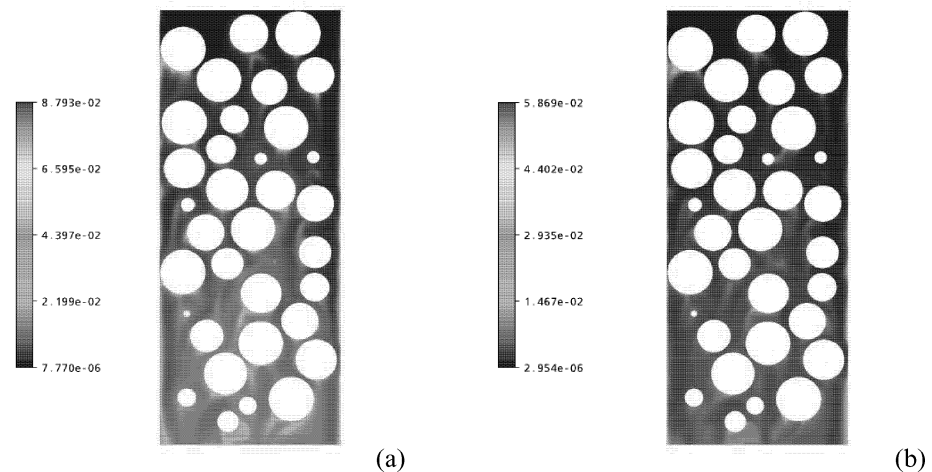


Figure 4. RTD (in seconds) obtained by the post-processing method for $\lambda = 3.78$; $Re_p=17.87$ (a) and $Re_p=45.08$ (b).

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. However, the post-processing method requires less computational power and time compared to the tracer method.

In the future, simulated RTD will be used to estimate the axial dispersion coefficient of the fixed bed reactors. The comparison with experimentally estimated dispersion coefficients will help to achieve a better validation of the RTD models.

6. References

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