Book of Abstracts
European Congress of Chemical Engineering (ECCE-6)
Copenhagen, 16-20 September 2007

CFD-based analysis of the wall effect on the pressure drop in packed beds

T. Atmakidis[a], E.Y. Kenig[a], E.S. Kikkinides[b]

a Department of Biochemical and Chemical Engineering, University of Dortmund, 44227 Dortmund, Germany
b Department of Engineering and Management of Energy Resources, University of Western Macedonia, 50100 Kozani, Greece

1. Summary

In this work, the influence of solid walls on pressure drop in packed beds is studied numerically for moderate particle/tube diameter ratios. Two different configurations are investigated, a regular configuration and a random one. The regular configuration follows the atomic face-centered cubic (FCC) structure in ideal crystals, while a ballistic deposition method is employed for the random configuration. To validate the simulation results, four experimental pressure drop correlations are used, namely the Ergun, the Carman, the Zhavoronkov and the Reichelt correlation. Simulation results for the regular configuration are in a good agreement with Carman correlation, while for the random configuration agreement with Zhavoronkov and Reichelt correlations is better.

Keywords: packed beds, CFD, pressure drop, channelling effect

2. Extended Abstract

Pressure drop is of crucial importance for the design and operation of packed bed reactors. There are several works, both experimental and numerical, approaching a correct description of the pressure drop in packed beds. However, the available information regarding the wall effect on pressure drop is contradictory (Eisfeld and Schnitzlein, 2001). On one hand, the wall introduces an additional pressure drop, just because of the wall friction. On the other hand, the pressure drop is reduced due to additional inhomogeneities close to the wall (channelling effect).
Eisfeld and Schnitzlein (2001) investigated the wall effect on pressure drop experimentally and developed a pressure drop correlation that was compared with existing correlations taken from the literature. An improved correlation was suggested based on experimental data, in which the wall effect was taken into account. Numerical simulations of fluid flow in packed beds for moderate particle/tube diameter ratios are useful for a better understanding of the phenomena caused by the influence of the wall.
In the present work, a commercial CFD tool CFX 10.0 by ANSYS Inc. is used to simulate the single-phase incompressible flow through fixed beds of spheres in arranged and random configurations. The arranged configurations follow the atomic face-centered cubic (FCC) structure in ideal crystals. To construct the random packing configuration of non-overlapping spherical particles, a ballistic deposition method is employed (Coehlo et al., 1997). This method is modified based on the Monte Carlo method. In order to place one spherical particle inside the tube, a relative large number of “test” particles are dropped and only the one whose final position is the lowest becomes a part of the stack. In Fig. 1, the void fraction and the number of particles is plotted against the number of the “test” particles. If the number of “test” particles, N, is high enough ($N>10^6$), random arrangements can be recovered. This method results in random 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).

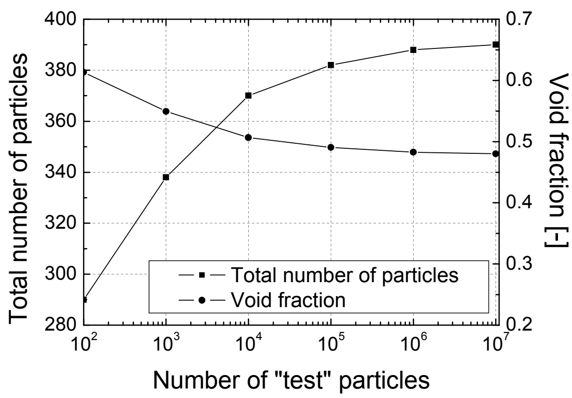

Figure 1 Void fraction and the number of particle as a function of the number of the “test” particles

The tube diameter/particle diameter ratio for the constructed geometries lies between 1 and 10. For this range of ratios, the wall effect on the pressure drop is significant. To simulate the fully developed flow neglecting inlet effects, periodic boundary conditions are imposed along the main flow direction. The use of periodic boundary conditions reduces the necessary computational domain length resulting in a substantial reduction of the required computer power and calculation time.

To validate the model, the pressure drop is calculated and compared with the most common correlations, namely, the Ergun, the Carman, the Zhavoronkov and the Reichelt correlations (see Eisfeld and Schnitzlein, 2001). In the last two correlations for the pressure drop, the influence of the wall is taken into account. In Fig. 2, the pressure drop simulation results are compared with the results obtained by the correlations for similar tube diameter/particle diameter ratio for both regular and random configurations. The dimensionless pressure drop is given by

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

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.

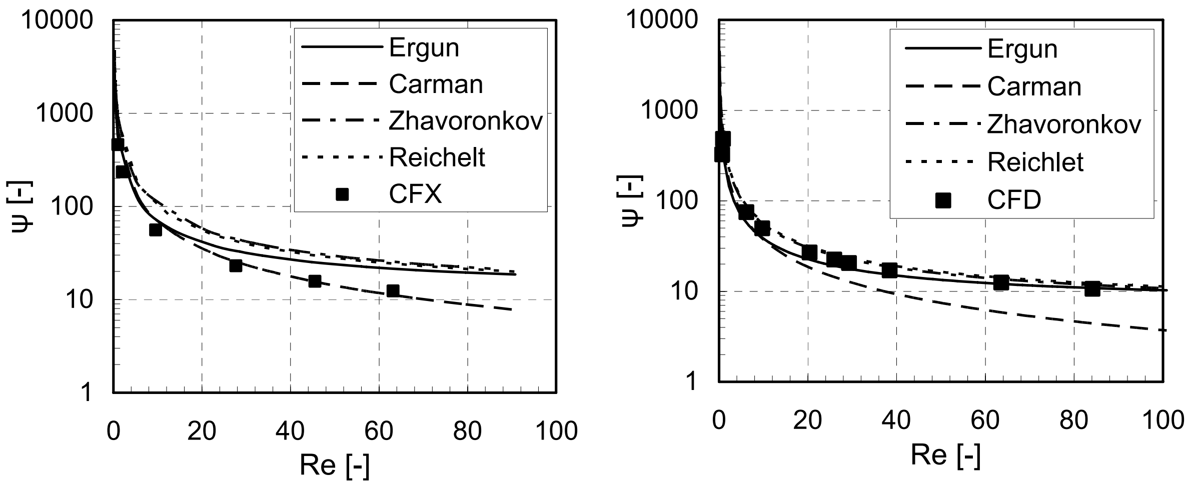

Figure 2 Pressure drop calculated by different methods for different particle Reynolds numbers, Re_p, for the regular (a) and the random (b) configuration.

Pressure drop simulations for the regular configuration agree better with Carman correlation, in which the influence of the wall is not considered. This unexpected result can be explained by the high channeling in the regular configuration. The local void fraction near the wall is very high leading to substantial local velocities. Due to this effect, the pressure drop in the regular configuration is reduced.

For the random geometry, simulation results agree better with the correlations that take into account the wall influence. The void fraction near the wall is here lower than in the regular configuration. Channeling also occurs for the random structures, but it is not as significant and structured as for the regular configuration. The random spherical packing arrangement is closer to the actual packed bed configurations, and hence, it should be taken into account for the correct description of the pressure drop.

References

Eisfeld, B. and Schnitzlein K., (2001) *Chemical Engineering Science*, 56, 4321–4329.

Coehlo, D., Thovert, J.F. and Adler, P.M., (1997) *Physical Review B*, 55, 1959-1978.

Kainourgiakis, M.E., Kikkinides, E.S. and Stubos A.K., (2002) *Journal of Porous Materials*, 9, 141-154.