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CFD modeling of pressure drop and drag coefficient in fixed beds: Wall effects

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ABSTRACT

Simulations of fixed beds having column to particle diameter ratio (D/d_p) of 3, 5 and 10 were performed in the creeping, transition and turbulent flow regimes, where Reynolds number ($d_p V_L \rho_L/\mu_L$) was varied from 0.1 to 10,000. The deviations from Ergun's equation due to the wall effects, which are important in $D/d_p < 15$ beds were well explained by the CFD simulations. Thus, an increase in the pressure drop was observed due to the wall friction in the creeping flow, whereas, in turbulent regime a decrease in the pressure drop was observed due to the channeling near the wall. It was observed that, with an increase in the D/d_p ratio, the effect of wall on drag coefficient decreases and drag coefficient nearly approaches to Ergun's equation. The predicted drag coefficient values were in agreement with the experimental results reported in the literature, in creeping flow regime, whereas in turbulent flow the difference was within 10–15%.

1. Introduction

Fixed beds having low D/d_p ratios (<10) are often used in the applications of exothermic and endothermic reactions in chemical industries. The flow complexities in these beds have so far prevented the detailed understanding of the flow structure in the interstices between the particles. This important subject has become amenable due to an increase in the computational power and the parallel developments in the numerical techniques. In the present work the effect of the column wall on the pressure drop and drag coefficient in fixed beds having different D/d_p ratios have been simulated using FLUENT 6.2 commercial CFD software.

1.1. Previous work

For the case of a fully developed flow in a fixed bed, Ergun (1952) has proposed the following semi-empirical correlation by linking the Kozeny–Carman equation for the creeping flow regime and the Burke–Plummer equation for the turbulent regime:

$$\frac{\Delta P}{L} = \frac{150\mu_L V_L}{d_p^2 \varphi^2}\frac{\in_S^2}{\in_L^3} + \frac{1.75\rho_L V_L^2}{d_p \varphi}\frac{\in_S}{\in_L^3}. \quad (1)$$

The above equation holds for the case of large D/d_p ratio (>15) where the condition of near uniformity prevails in the void fraction throughout the bed. For the case of $D/d_p < 15$, the voidage tends to be greater near the wall than in the bulk region. Under these conditions a significant deviation in pressure drop occurs as compared to Eq. (1) (Di Felice & Gibilaro, 2004; Eisfeld & Schnitzlein, 2001; Foumeny, Benyahia, Castro, Moallemi, & Roshani, 1993; Mehta & Hawley, 1969; Nield, 1983; Reichelt, 1972).

Various researchers have addressed the effect of wall on the pressure drop in the low D/d_p ratio beds. Earlier studies have been performed by Carman (1937) and Coulson (1949) under creeping flow conditions, and describe the wall effects by including the surface area of the column in the definition of the drag coefficient. Mehta and Hawley (1969) have studied the wall effects on pressure drop in packed beds having $7 < D/d_p < 91$ and Reynolds number less than 10. Similar type of experiments have been carried out by Chu and Ng (1989) in fixed beds having D/d_p ratio 2.9 to 24 and $Re < 5$. These experiments have shown that the pressure drop (ΔP) behaves according to Eq. (1) only when $D/d_p > 15$. Below this value, at every Re, ΔP was found to increase (compared with Eq. (1)) with a decrease in the D/d_p ratio. In the turbulent flow regime the pressure drop in low D/d_p ratio fixed beds having spheres, cylinders and rings has been measured by Leva (1947). Foumeny et al. (1993) have made measurements in the turbulent region with D/d_p ratio in the range of 3–24. In these cases also, the pressure drop was found to follow Eq. (1) when $D/d_p > 15$. Below this value, at any Re, the pressure drop was found to decrease with a decrease in the D/d_p ratio.

These wall effects have been comprehensively reviewed by Eisfeld and Schnitzlein (2001) by analyzing all the experimental results in the published literature. The authors have confirmed

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Nomenclature

A_P	surface area of the particle (m^2)
C_D	drag coefficient including both hydrodynamic drag force on particles and the column wall
$C_{\varepsilon 1}$	model parameter in ε equation
$C_{\varepsilon 2}$	model parameter in ε equation
C_μ	model parameter for k–ε model
D	column diameter (m)
d_p	particle diameter (m)
F_D	drag force on single particle, (kg m/s^2)
k	turbulent kinetic energy (m^2/s^2)
L	length of the bed (m)
P_i	pressure (N/m^2)
$\langle P_i \rangle$	time averaged pressure (N/m^2)
ΔP	pressure drop (N/m^2)
Re	Reynolds number ($d_p V_L \rho_L / \mu_L$)
S_p	surface area of particles (m^2)
S_W	surface area of wall (m^2)
u_i	instantaneous velocity of component i, where i = 1, 2, 3 corresponds to radial, axial and tangential component of velocity (m/s)
$\langle u_i \rangle$	time average of velocity (m/s)
V_L	superficial velocity (m/s)
V_p	volume of the particle (m^3)

Greek symbols

ε	energy dissipation rate (m^2/s^3)
$\in_L$	voidage of bed
$\in_S$	fractional solid hold-up
μ_L	molecular viscosity of fluid (kg/(m s))
ρ_L	density of fluid (kg/m^3)
ν	kinematic viscosity (m^2/s)
ν_t	eddy viscosity (m^2/s)
φ	shape factor
σ_k	model parameter
σ_ε	model parameter

Subscript and superscript

i, j, k	co-ordinates in generalized form with value 1, 2 and 3 corresponding to radial, axial and tangential direction
L	liquid phase
S	solid phase

the observations of Mehta and Hawley (1969), Reichelt (1972) and Foumeny et al. (1993) in the creeping and turbulent regimes respectively. Further they conclude that the Reichelt (1972) correlation, which corrects the Ergun's equation for wall effects, is the most promising one. The correlation is given below:

$$\frac{\Delta P}{L} = \frac{K_1 A_W^2 \mu_L V_L}{\varphi^2 d_p^2} \frac{\in_S^2}{\in_L^3} + \frac{B_W \rho_L V_L^2}{d_p \varphi} \frac{\in_S}{\in_L^3}, \tag{2}$$

where

$$A_W = 1 + \frac{2}{3(D/d_p)(\in_S)}, \tag{3}$$

$$B_W = \frac{1}{\left[k_1 (d_p/D)^2 + k_2\right]^2}. \tag{4}$$

The coefficients K_1, k_1 and k_2 have been obtained by fitting the experimental data. For spheres, they proposed, K_1 = 154, k_1 = 1.5 and k_2 = 0.88 and for cylinders K_1 = 190, k_1 = 2 and k_2 = 0.77. From the foregoing discussion it may be emphasized that the work of Eisfeld and Schnitzlein (2001) is empirical in nature.

For predicting the wall effects on the pressure drop in low D/d_p ratio fixed beds a two zone (wall and bulk zones) model have been proposed by Di Felice and Gibilaro (2004). Their model overpredicts the experimental results of Leva (1947) and Foumeny et al. (1993) in the turbulent flow regime.

As regards to mathematical modeling, CFD simulations give very detailed flow information in the complex geometry like fixed beds. Dalman, Merkin, and McGreavy (1986) began the 2D CFD simulations by considering only two particles and resolved the flow pattern around the particles for Reynolds number up to 200. Lloyd and Boehm (1994) extended the CFD simulation for the case of eight spheres in a row. In this study the influence of the sphere spacing on the drag coefficient was investigated. However, as expected, 2D simulations were not sufficient to resolve the flow complexities. Nijemeisland and Dixon (2004) have reported 3D simulation (using FLUENT) of fixed bed of D/d_p = 4 and 72 particles. Guardo, Coussirat, Larrayoz, Recasens, and Egusquiza (2005) have investigated the wall-to-fluid heat transfer and pressure drop for the case of D/d_p = 3.92 (44 particles) and over a Reynolds number (Re) range 100–1000.

Calis, Nijenhuis, Paikert, Dautzenberg, and van den Bleek (2001) have simulated the pressure drop and drag coefficient in square channels with particles, having D/d_p ratio in the range of 1–2 (8–40 particles) by using CFX 5.3 commercial CFD software. The values obtained from CFD simulation were shown to agree with the experimental measurements on laser Doppler anemometer (LDA). Though this study has not explained the wall effect in low D/d_p fixed beds, it serves as a good beginning. Recently Reddy and Joshi (2008) have predicted the wall effects in fixed and expanded beds having only one D/d_p ratio of 5.

From the foregoing discussion, there is a clear need to understand the wall effects in fixed bed having low D/d_p ratios and over a wide range of Reynolds number (0.1–10,000) covering creeping, transition and turbulent regimes by resolving the flow around each individual particle. The present "shorter communication" is in the continuation of our earlier work (Reddy & Joshi, 2008) where, the effect of wall at one D/d_p ratio of 5 has been studied. In this communication, the effect of wall on the pressure drop and drag coefficient in fixed beds having different D/d_p ratios of 3, 5 and 10 has been presented. However, the available computational resources restricted the simulations for D/d_p ratios up to 10.

2. CFD modeling

2.1. Computational geometry and grid generation

All computational geometries were generated by using bottom-up technique (volumes were generated from surfaces and edges) by using commercial software GAMBIT 2.0.4 (Reddy & Joshi, 2008). In all the fixed bed geometrical models having the particle size of 25.4 mm, the total number of particles and the height of the bed were varied for covering three different D/d_p ratios (3, 5 and 10). In order to study the effect of D/d_p ratio on the pressure drop and drag coefficient all the fixed beds (D/d_p = 3, 5 and 10) were constructed in such a way that the void fraction remains constant (0.439). It is important that only one variable is considered at one time. In all geometries, surface of the all particles are well refined (up to 1200 surface nodes) for getting accurate predictions. In the present study the simulations were restricted to particle bed, as a result, the distributor at the inlet and the bed limiter at the outlet have not been simulated. For simplicity, the inlet boundary condition was considered to be a flat velocity profile, whereas the