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Study of flow through a packed bed using discrete element method and computational fluid dynamics

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ABSTRACT

Packed beds find wide applications in chemical industries. In this paper, a Discrete Element Method (DEM) – Computational Fluid Dynamics (CFD) approach has been adopted to predict the flow profile in the bed for different diameter of the bed/diameter of the particle. The randomly packed bed was created using the DEM technique. The radial voidage of the bed was calculated using the Monte Carlo integration method. The radial voidage showed an oscillating pattern up to approximately 4–5 particle diameter from the wall, which was validated with the experimental data reported by several researchers. The flow studies through these packed beds were carried using single-phase laminar flow model. The flow followed a similar oscillating pattern as the radial voidage. The numerical results were validated with experimental data. Preliminary studies to predict the residence time distribution has also been carried out using the multi-species transport model, which was also experimentally validated. The study suggests that DEM and CFD simulation can predict the flow behaviour as well as Residence Time Distribution (RTD) in a packed bed quite satisfactorily without the need to carry out experiments, which would be environmental friendly.

1. Introduction

Packing of particles in three-dimensional space has been of great interest in various areas of industrial applications. Determination of permeability in porous media [1] heterogeneous catalysis [2]; separation process such as chromatography etc., deal with packed beds. Coarse packed beds have been used for denitrification of waste water [3] as well as CO_2 sequestration [4]. The density of a packed bed depends on the arrangement of the particles in the bed. In 1611, Kepler conjectured that the closest packing could be achieved with face centred cubic lattice in the case of three dimensional (3D) packing with an occupation coefficient of ~0.74. The proof of Kepler's conjecture for 3D packing has been given by Thomas C. Hales [5]. In packed beds, the particles are usually randomly arranged, and the maximum possible value of the occupation coefficient, for random close packing of mono dispersed spherical particles, in the case of 3D is approximately 0.64. Random Close Packing (RCP) for monodisperse sphere is well explained mathematically and the density varies in a very narrow range [6]; which can be reproduced [7]. When carrying out numerical simulations to study the flow pattern, packed beds are often represented by randomly arranged spherical particles.

To envisage the mechanical behaviour of granular materials by numerical simulation, the discrete element method (DEM) has often been used. This can be done by calculating the displacement of the particles either on a dynamical basis [8–11], or according to a quasi-static approach [11–16].

The flow study in packed beds was initiated with the creeping flow studies by Darcy in 1856. Since then, many experimental studies as well as models have been developed to study the pressure drop in packed beds. Ergun [17] and Ergun and Orning [18] have obtained a correlation for estimating the pressure drop in a bed of solids based on a number of experiments that they carried out for various types of packing, fluid velocities and void fractions, which is given as

$$\left(\frac{(-\Delta P \boldsymbol{g\rho})}{\phi^2}\right)\left(\frac{d}{l}\right)\left(\frac{\boldsymbol{\varepsilon}^3}{1-\boldsymbol{\varepsilon}}\right) = 150\frac{\boldsymbol{\mu}(1-\boldsymbol{\varepsilon})}{d\phi} + 1.75 \quad (1)$$

where d is the particle diameter, ϕ is the mass flux, ε is the voidage and l is the characteristic length of the bed. The ratio of bed diameter to particle diameter was large (~25) in the experiments conducted by Ergun. When the diameter of the column is much larger than the particle diameter, the wall will have little effect on the characteristic length. For small D/d ratios, the wall

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will have a considerable effect on the flow behaviour. Mehta and Hawley [19] have included the wall effect for small D/d (bed diameter/particle diameter) ratios (specifically in the range of 1–7). The modified Ergun correlation given by them is,

$$\left(\frac{(-\Delta P \boldsymbol{g}\boldsymbol{\rho})}{\phi^2}\right)\left(\frac{d}{l}\right)\left(\frac{\boldsymbol{\varepsilon}^3}{1-\boldsymbol{\varepsilon}}\right)\left(\frac{1}{M}\right) = 150\frac{\boldsymbol{\mu}(1-\boldsymbol{\varepsilon})M}{d\phi} + 1.75 \quad (2)$$

where the hydraulic radius, R_h is defined as,

$$R_h = \frac{\boldsymbol{\varepsilon} d}{6(1-\boldsymbol{\varepsilon})M} \quad (3)$$

which can be compared to Kozeny's equivalent diameter factor, d_m [20,21], but with an extra factor M, that incorporates the wall effect. M is defined as,

$$M = 1 + \frac{4d}{6D(1-\varepsilon)} \quad (4)$$

Liu et al. [22] have also reported a modified form of Ergun's equation, which takes into account the wall effect.

Experimental studies on the velocity profile at the outlet for packed beds have been carried out by various researchers to understand the effect of the wall on the flow [23–25]. Maximum velocity was near the wall, and the flow followed an oscillating pattern with the amplitude decreasing towards the centre. Various mathematical models for predicting velocity distribution in a packed bed have been reported by several authors [23–28]. Ziółkowska and Ziółkowski [23] as well as Bey and Eigenberger [24] have used effective viscosity, which is an empirical parameter based on the geometry, aerodynamics and physical properties, for predicting the velocity profile. In their recent work Ziółkowska and Ziółkowski [29] included the radial dispersion in the model for predicting the velocity profile. Various experimental techniques have been adopted to study the radial voidage variation in packed beds [30–35], which are destructive in nature. These studies showed that the maximum radial voidage is at the wall, with an oscillating pattern towards the centre, which becomes almost constant after approximately 4–5 particle diameter from the wall. The radial voidage was also studied by various other methods, which were non-destructive in nature [36–40]. These studies also show the same damped oscillatory pattern for the radial voidage; however, Stanek and Eckert [38] reported that the damped oscillation was observed up to 6 particle diameter. Several empirical correlations have also been reported for predicting the average voidage variation as well as, radial voidage variations as a function D/d ratios [26–28].

Some simulation studies have been carried out to study the flow behaviour in packed beds, but these are limited to D/d ratio between 2 and 6, and with a maximum of 2000 particles [41–46]. These approaches include CFD as well as lattice Boltzmann method (LBM) simulations. Zeiser et al. [41] used LBM to study the gas flow behaviour in a catalyst filled tube. The packing study was done by the Monte Carlo method. The radial voidage obtained was compared with that obtained by Bey and Eigenberger [24] and the deviation was found to be large in the central region of the bed. Though the Monte Carlo method accounts for the randomness in a bed, it does not account for the particle-particle interaction under gravity. They have reported that they have used at least 40 spheres for the packed bed and D/d ratio of 5 and 6. Freund et al. [42] used the Monte Carlo method for the random generation of spheres and then translated them in the direction of gravity for dense packing. The flow simulations were next carried out using LBM. The study was performed on a single bed of D/d ratio 5. Calis et al. [43] have used a simulation algorithm to generate a packed channel with a square cross-section for the channel to particle diameter ratio varying from 1 to 2. The CFD simulations were carried out to study the flow behaviour in the channel considering the assembly of spheres as a wall with a maximum of 16 particles. Nijemeisland and Dixon [44] generated a packed bed using ordered packing with 44 spheres of size 2.54 cm and for D/d ratio of 2. CFD studies were carried out to study the convective heat transfer in the bed. Behnam et al. [45] have recently reported CFD simulations studies on heat transfer in a packed bed. The packed bed was generated using "soft-sphere" algorithm. The particles were generated randomly throughout the bed and overlaps were reduced, in the absence of gravity, this led to low packed bed voidage than usual. Then, a gravitational force was applied to make the bed dense. The bed was generated for D/d ratios of 3.96, 5.96 and 7.99 with a maximum of 400 particles. Zaman and Jalali [46] have studied hydraulic permeability in porous media generated by hard sphere algorithm using CFD. The study was performed in a cubic box with lower range of porosities and varying the number of particles between 20 and 2000 particles.

Table 1
Bed parameters (height = 0.225 m, particle diameter = 0.015 m).

Bed diameter(m)	D/d ratio	No. of particles packed
0.054	3.6	140
0.084	5.6	381
0.112	7.5	645
0.142	9.5	1063
0.152	10.1	1281
0.242	16.1	3287
0.302	20.1	5141

In this paper, flow behaviour through randomly packed beds has been studied by DEM-CFD coupling. The randomly packed bed has been generated using the DEM technique with spheres of 1.5 cm diameter and D/d ratio varying between 3 and 20. Packed bed reactors for denitrification, which is basically a coarse media filter, use a minimum particle size of 1.5 mm [3]. The media used are stone, gravel, granular activated carbon etc. Also, CO_2 sequestration in packed bed of limestone preferably use particle in the size range of 2–30 mm, to avoid significant entrainment losses of limestone particles from the bed [4]. In this study, CFD simulations for the DEM generated packed beds have been carried out to study the velocity profile for D/d ratios in the range 3–16, which have been validated experimentally. Also, preliminary studies on residence time distribution (RTD) in a packed bed using CFD have been attempted for D/d ratio of 5.6, which has been experimentally validated.

2. Experimental method

The experiments were carried out in PVA columns of varying diameters. Fig. 1a shows the experimental setup of the packed bed with the collector underneath it and a nozzle maintained at a height so that the liquid is sprayed uniformly across the entire cross-sectional area of the bed. Table 1 lists the different D/d ratio of the beds used in the study. Particles (glass beads) of 1.5 cm diameter and with an average density of ~2700 kg/m^3 were used in all the experiments. The standard deviation in the diameter of particles was approximately 2%. Fig. 1b shows the co-axial cylindrical collector used for collecting water at different radial distance. The collector was fabricated using galvanized iron sheets. A sieve of 10 mm mesh size (Fig. 1c) was used to hold the packed bed and to avoid any impact of the sieve on the flow behaviour.

The packing was done by drop method, with uniform vertical vibration, to generate a dense packing. For the flow study, a specialized nozzle was used, which sprays at an angle of 90° and maintains uniform distribution across the cross-section. A monoblock AC pump (TULLU Pump Corporation) was used to maintain constant flow rate, which had a throughput of 1680 Lh^{-1}. The