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Pressure drop investigations in packings of arbitrary shaped particles

K. Vollmari, T. Oschmann, S. Wirtz, H. Kruggel-Emden *

Ruhr-Universitaet Bochum, Universitaetsstrasse 150, D-44780 Bochum, Germany

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ABSTRACT

Unstructured packings consisting of arbitrary shaped particles are widely used in chemical, biochemical and petrochemical industries as well as in energy technology. In packings passed through by a fluid, pressure drops are of key concern and can be derived experimentally, calculated by empirical correlations or by numerical approaches. Among numerical approaches either resolved flow simulations or porous approaches are feasible. In the latter approach large systems can be addressed at reasonable computational expense. The fluid velocity is addressed as a spatially averaged quantity per fluid cell which is larger than a single particle. Information on the porosity must be provided by either experimental techniques or particle based methods such as the discrete element method (DEM). The DEM can be coupled with computational fluid dynamics (CFD) to a combined DEM–CFD approach and is then applicable to systems involving arbitrary shaped particles. As flow is not resolved in porous approaches information on the pressure drop must be provided by suitable submodels e.g. the combination of the drag force model by Di Felice (Int. J. Multiph. Flow. 20 (1994) 153–159 [1]) and the drag coefficient model by Hölzer and Sommerfeld (Powder Technol. 184 (2008) 361–365 [2]). As there is an ongoing discussion regarding the validity of these combined submodels, pressure drops in packings of spherical and non-spherical particles are derived by carefully performed experimental investigations as a verification. Numerically obtained results from the DEM–CFD are benchmarked against the experiments and available empirical correlations for the pressure drop. Results are in very good agreement for spheres. For complex shaped particles DEM–CFD simulations can be very flexibly applied. Simulations are generally in good agreement with experiments depending on the particle shape and size and are often better than empirical correlations which are usually tailored towards certain shapes and therefore limited in their usability.

1. Introduction

Unstructured packings consisting of arbitrary shaped particles are widely used in processes such as absorption, stripping and catalysis [3] as well as for heat storage/cooling or processes such as gasification, pyrolysis and carbonization [4]. Particles in packings can be of random shape and size such as rock, coal or wood chips or of uniform well defined geometry as in pebble bed reactors or in packed columns.

When a fluid passes through a packing it flows through a network of voids and channels formed by the particles resulting in an overall fluid pressure drop. Usually a packing can be characterized by few parameters such as the particle size and shape, the packing depth and width and the porosity. In case that a packing is confined by vessel walls interactions with the walls can become relevant especially for small bed width to particle size ratios resulting in non-uniform flow profiles. Two phenomena are observable: permeability close to the walls is enhanced and viscous friction with the walls can become relevant. Both phenomena in combination have a strong non-linear effect on the overall pressure drop in the packing [5]. For width to particle diameter ratios larger 10 (wide packings) usually low, for ratios smaller than 10 (narrow packings) significant influence is reported [6]. Understanding the resulting flow as well as pressure drop in wide and narrow packings is essential with regard to the scale-up and for the optimization of operation parameters of processes related to chemical, biochemical and petrochemical industries as well as energy technology.

When only the pressure drop is of interest a large number of empirical correlations is available which predict the overall pressure drop in the bed mostly based on parameters involving porosity, particle characteristics (shape, size, surface), fluid velocity, fluid density, fluid viscosity, bed depth and width [7–17]. Most correlations are suited for spherical particles only [7–9,11–17] — few correlations are applicable to complex shaped particles, where either geometrically equivalent spherical particles are considered [7,13] or particles have to be of a well-defined uniform shape and size [4,6,11,12]. Furthermore, experimental investigations can be performed especially if existing correlations are doubted to be sufficiently accurate [18], more detailed information needs to be gained on the fluid flow than just the pressure drop [19] or heat and mass transfer as well as reactions need to be addressed simultaneously [20,21].

In contrast to correlations and experimental investigations several numerical approaches are available to investigate the flow within

* Corresponding author. Tel.: +49 234 32 27362; fax: +49 234 32 14 227.
E-mail address: Kruggel-emden@leat.rub.de (H. Kruggel-Emden).

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particle packings mostly based on computational fluid dynamics (CFD). Mainly two different approaches are available: the resolved flow approach and the porous approach [22].

In the resolved flow approach fluid flow around individual particles is represented in detail. Thereby, no closures for the pressure drop in the form of empirical correlations are required. The pressure drop results from the detailed representation of viscous friction within the network of channels and voids inside the packing. Obtained results are of high accuracy but computationally very demanding and therefore restricted to model-type systems. Methods applicable involve the Lattice Boltzmann method (LBM) which instead of discretizing the Navier–Stokes equations relies on the Boltzmann equation and kinetic theory [23–25]. In contrast to the LBM, finite-volume-methods (FVM) can be used for the approximation of the Navier–Stokes equations which usually rely on surface adapted meshes. Topics addressed by resolved flow investigations in recent years comprise of detailed flow analysis [26–28], multiphase flow problems [29], wall effects [30,31], heat transfer [32–34], as well as mass transfer and reactions [35,36].

In the porous approach the fluid velocity is addressed as a spatially averaged quantity per fluid cell which is larger than a single particle. The pressure drop is calculated based on the global averaged or local porosity which has to be obtained by e.g. experimental techniques such as e.g. 3D MRI [37] or numerical methods such as the discrete element method (DEM) [38–40] which is addressed later in more detail. In the latter method the individual particle orientation can be considered in case of complex shaped particles [41]. DEM approaches can be transiently coupled to the CFD and as a combined DEM–CFD be applied to moving particle systems [41,42] or systems involving heat and mass transfer [43,44].

Pressure drop calculations involving complex shaped particles based on the DEM–CFD method are yet not widely established. So far DEM–CFD approaches involving non-spherical particles have been mainly applied to the dynamic simulation of moving or fluidized systems [41,45]. Regarding the validity of the approach there is an ongoing discussion about its applicability and limitations [41,46] as it combines single particle force models applicable for complex shapes [2] with voidage corrections established in the context of systems of spherical particles [1]. A refined voidage function including flow velocity and local porosity was proposed recently for systems of spheres [47]. Note that the voidage function [47] results in similar values as [1] for densely packed beds. To apply the DEM–CFD reliably to systems of complex shaped particles detailed investigations are necessary regarding the applicability of the combination of the submodels [1,2]. In contrast to the resolved flow approach the porous approach based on the DEM–CFD offers the opportunity to address industrial scale packings of arbitrary shaped particles and additionally allows to model heat and mass transfer and reactions in one framework which by far exceeds capabilities of simple empirical pressure drop correlations today available in large numbers.

One step towards a verification of the porous approach based on the DEM–CFD is intended through this investigation. The DEM–CFD is applied for the calculation of pressure drops in packings of spherical and non-spherical particles of varying sizes in the present investigation. To prove the validity of the DEM–CFD involving submodels [1,2] a comparison against carefully performed experimental investigations is performed for a model scale fixed bed. Additionally, available correlations are reviewed and benchmarked against numerical and experimental results.

2. Methodology

The investigations of this study focus on the verification of the porous approach involving the DEM–CFD method in which flow around individual particles is not resolved for packed beds of arbitrary shaped particles based on pressure drop predictions. As reference multiple empirical correlations for the determination of the pressure drop of packed beds for spherical and non-spherical are considered as well as carefully performed experiments. In the following two subsections existing pressure drop correlations are reviewed and the applied porous approach using the DEM–CFD is outlined.

2.1. Correlations for the pressure drop calculation in fixed beds

The following subsection gives a summary of correlations available for different particle shapes involving spheres and some non-spherical shapes.

2.1.1. Correlations for spherical particles

The most frequently used pressure drop correlation for packed beds has been devised by Ergun [7] as it is applicable over a wide range of flow regimes. As many factors determine the pressure drop which are not always easy to obtain through experimental measures, Ergun identified the four most influential as (1) the fluid velocity, (2) fluid density and viscosity, (3) porosity and (4) the particle diameter, shape and surface. To simplify the calculation of the pressure drop a capillary bed model has been devised under the assumption that the fluid flow through a packed bed is comparable to that of flow through a capillary. Results from the capillary model are improved by accounting for correction factors gained from a multitude of experiments. The Ergun-equation is expressed through two terms, one for the viscous energy losses with the constant 150 and one for the kinetic energy losses with the constant 1.75. It can be written as follows:

$$\frac{\Delta p}{L} = 150 \cdot \frac{(1-\varepsilon)^2}{\varepsilon^3} \cdot \frac{\eta_f \cdot w_f}{d_p^2} + 1.75 \cdot \frac{1-\varepsilon}{\varepsilon^3} \cdot \frac{\rho_f \cdot {w_f}^2}{d_p} \tag{1}$$

with the bed height L, the porosity ε, the dynamic viscosity of the fluid η_f, the superficial velocity w_f and the particle diameter d_p. The Ergun-equation was chosen as the reference equation of this study for both the DEM–CFD simulations and correlations and is compared to newer methods for predicting the pressure drop. The Ergun-equation neglects wall effects and is therefore applicable for column diameter D to particle diameters d_p of $\gg 10$ [17].

As especially in small reactors the wall friction plays an important role in the total pressure drop of a system, some efforts have been made to incorporate these effects into the Ergun-equation. One of the first extension considering wall effects, dates back to Metha and Hawley [8]. They suggested the application of a correction factor to both linear terms of the Ergun-equation so that it appears as:

$$\frac{\Delta p}{L} = 150 \cdot \frac{(1-\varepsilon)^2}{\varepsilon^3} \cdot \frac{\eta_f \cdot w_f}{d_p^2} \cdot M^2 + 1.75 \cdot \frac{1-\varepsilon}{\varepsilon^3} \cdot \frac{\rho_f \cdot {w_f}^2}{d_p} \cdot M. \tag{2}$$

The correction factor M depends on the ratio of the particle diameter d_p to column diameter D as:

$$M = 1 + \frac{4 d_p}{6D(1-\varepsilon)}. \tag{3}$$

In case of a rectangular geometry the column diameter D is given by the hydraulic diameter. M has been determined through experiments under such conditions that the wall effect is of importance $7 < D/d_p < 91$. Metha and Hawley suggest using their correlation for column diameter D to particle diameter d_p ratios of >7 instead of Eq. (1). Foumeny et al. [9] expanded the correlation to be applicable for a wider D/d_p ratio as they found great deviations between experimental and calculated data at small D/d_p ratios of 3.5. They replaced the coefficients defined by Ergun leading to the following equation which is reliable for $3.23 < D/d_p < 23.8$:

$$\frac{\Delta p}{L} = 130 \cdot \frac{(1-\varepsilon)^2}{\varepsilon^3} \cdot \frac{\eta_f \cdot w_f}{d_p^2} + \frac{D/d_p}{2.28 + 0.335 \cdot (D/d_p)} \cdot \frac{1-\varepsilon}{\varepsilon^3} \cdot \frac{\rho_f \cdot {w_f}^2}{d_p}. \tag{4}$$