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On hydraulic permeability of random packs of monodisperse spheres: Direct flow simulations versus correlations

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ABSTRACT

Hydraulic permeability is studied in porous media consisting of randomly distributed monodisperse spheres by means of computational fluid dynamics (CFD) simulations. The packing of spheres is generated by inserting a certain number of nonoverlapping spherical particles inside a cubic box at both low and high packing fractions using proper algorithms. Fluid flow simulations are performed within the interparticulate porous space by solving Navier–Stokes equations in a low-Reynolds laminar flow regime. The hydraulic permeability is calculated from the Darcy equation once the mean values of velocity and pressure gradient are calculated across the particle packing. The simulation results for the pressure drop across the packing are verified by the Ergun equation for the lower range of porosities (<0.75), and the Stokes equation for higher porosities (~ 1). Using the results of simulations, the effects of porosity and particle diameters on the hydraulic permeability are investigated. Simulations precisely specified the range of applicability of empirical or semi-empirical correlations for hydraulic permeability, namely the Carman–Kozeny, Rumpf–Gupte, and Howells–Hinch formulas. The number of spheres in the model is gradually decreased from 2000 to 20 to discover the finite-size effect of pores on the hydraulic permeability of spherical packing, which has not been clearly addressed in the literature. In addition, the scale dependence of hydraulic permeability is studied via simulations of the packing of spheres shrunk to lower scales. The results of this work not only reveal the validity range of the aforementioned correlations, but also show the finite-size effect of pores and the scale-independence of direct CFD simulations for hydraulic permeability.

1. Introduction

The study of fluid flow through random porous media has a significant role in related fields of science and technology. It has been extensively addressed in the literature [1–4]. Flow through porous media has a wide range of applications in chemical engineering, ceramic engineering, mechanical engineering, food technology, the petroleum industry, separation processes, the paper industry, geophysics and environmental engineering and many other technological processes [5–8]. Some processes and devices associated with the study of flow through porous materials include filtering, drying, fuel cells, insulators, melting and solidification of binary mixtures, enhanced heat transfer by surface modification, oil and gas flow in reservoirs, natural gas production, enhanced oil production, the extraction of oil from porous rocks, chromatography, ground water flow, contamination migration in groundwater, water percolation in snow, soil cleanup by steam injection, the spread of hazardous waste in soils, and the degradation of building materials such as concrete.

Darcy [9] was the first one who measured the bulk resistance of a solid matrix to incompressible fluid flow. His experiment led to the introduction of hydraulic permeability which is the most important characteristic parameter of a porous

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matrix. The hydraulic permeability, K, is defined by the Darcy's law as

$$K = -\frac{\mu u}{\partial P/\partial x}, \tag{1}$$

where u is the fluid superficial velocity, μ is the viscosity of the fluid and $\partial P/\partial x$ is the pressure gradient in the direction of flow. Darcy's law creates a linear relationship between the velocity and pressure gradient, which is the alternative to the assumption of the linear proportionality of drag and velocity. This is a characteristic of the Stokes flow. In other words, this equation is valid for small velocities, when the Reynolds number based on the pore size is less than unity, where the viscous forces are dominant over the inertial forces. According to Eq. (1), the hydraulic permeability is a criterion for the flow conductance of the medium. While permeability is independent of the interstitial fluid properties, it depends on the geometric properties of the medium such as porosity (or void volume fraction), ε, average pore size and tortuosity.

The estimation of hydraulic permeability for porous media still remains a challenging issue from both theoretical and experimental points of view [10]. A great deal of effort has been made to find a relationship which can accurately predict the permeability based on the above-mentioned geometric properties. There are many correlations which have been proposed to simply relate permeability to porosity and a pore size parameter such as the particle diameter in the packing of spherical particles. The most well-known correlation was proposed by Kozeny [11] and Carman [12] in which the concept of hydraulic radius was used in a semiheustristic model and is usually called the Carman–Kozeny theory [13]. Rumpf and Gupte [14] presented another correlation for packed beds of spherical particles with a narrow range of distribution in size which has a better consistency with the experimental results in the range of porosities from 0.35 to 0.70. Brinkman [15] introduced a self-consistent estimation for the permeability of porous matrices. After that, Childress [16], Howells [17], and Hinch [18] obtained completely convergent cluster type expansions for the beds of randomly dispersed single size spheres [19].

In the present work, the permeability of a random packing of spheres is precisely calculated in various simulations corresponding to different porosities via solving Navier–Stokes equations for the interstitial flow through particle packing. Moreover, the effect of the number of spheres on the hydraulic permeability is investigated at any porosity inside the containing box with fixed dimensions. Simulations are also performed for downscaled packings to investigate the effect of the pores' scale on hydraulic permeability. The comparison of results of simulations for hydraulic permeability with those predicted by three common correlations is another aim of this work.

2. Methods

Our simulation method relies on three major steps which include the generation of particle packings with the given parameters, the recreation of the packing geometry and corresponding grids for computational fluid dynamics (CFD) calculations, and finally solving the governing equations of interstitial flow in the particle packing.

2.1. Generation of packings

Monodisperse spherical random packings are built in a cubic container with a variety of given porosities. The porosity of packings varies from 0.45 to 0.95 with an increment of 0.05. In addition, two extreme packings are represented by the porosities of 0.99 and 0.38. In order to study the effect of the number and size of particles on hydraulic permeability, a number of packings consisting of a different number of spheres is generated. At any porosity, seven packings with the number of spheres varying from 20 to 2000 are created. Obviously, lowering the number of spheres in the system increases the size of spheres by noting that the size of container is kept constant. The relation between the spheres' diameter d, porosity ε and the number of particles N is

$$d = \left(\frac{6\,(1-\varepsilon)}{\pi N}\right)^{1/3}. \tag{2}$$

The generation of spherical packings is performed using either a Monte Carlo (MC) approach for dilute packings ($\varepsilon > 0.70$), or molecular dynamics (MD) simulation approach for dense packings ($\varepsilon < 0.70$). Here, the MC approach simply refers to the random insertion of spheres inside the cubic container so that the existence of nonoverlapping spheres is guaranteed. In dilute packings, the MC algorithm of the packing generator code inserts particles randomly inside the box. Meanwhile, the nonoverlapping condition must be satisfied between any newly generated sphere and all previously generated spheres until the given number of spheres is inserted. However, this method is extremely inefficient as the porosity drops below 0.70. For the porosities less than 0.70, the MD approach for densification of hard sphere packings is employed which was presented by Jalali and Li [20]. The packing generator code generally assigns the size and position of spheres based on the given values for porosity and the number of spheres in a cubic box with unit dimensions. The lateral sides of the box are subjected to the periodic boundary condition [21]. The MD algorithm for the densification of spherical packings uses a hard sphere method in which the size of spheres grows every time step given as an input of the code. The packing of hard spheres ends up with a disordered array of spheres when the densification rate is high enough. Further details about the computational method can be found in Jalali and Li [20]. The densification of spherical packing is stopped once the targeted porosity is achieved.