



Fluid particle interaction in packings of monodisperse angular particles

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ABSTRACT

Understanding fluid flow in granular materials is essential for many engineering applications, including petroleum recovery, groundwater movement and embankment stability. This study investigates the influence of particle angularity on permeability and fluid-particle interaction forces. A random shape generator based on spherical harmonics is used to create irregular-shaped particles with different levels of angularity. Granular packings of uniformly sized (monodisperse) particles are then constructed with the discrete element method (DEM), and pore-scale computational fluid dynamics (CFD) simulations are used to determine the flow fields and the resulted fluid-particle interaction. The more angular particle assemblies thus generated are less permeable, and their fluid-particle interaction forces are higher. However, angularity has limited influence on flow rate distribution and flow tortuosity. The influence of angularity is localized. An increase in angularity generates a larger variance of the pressure distribution on the particle surfaces, thus increasing the pressure component of the fluid-particle interaction force.

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1. Introduction

Fluid flow in granular materials has two primary impacts on many engineering processes. Firstly, torturous flow paths exert resistance to fluid flow and determine the production of hydrocarbons in oil and gas reservoirs [1] and groundwater flow in aquifers [2]. Secondly, fluid flow generates fluid-particle interactions on individual particles, which can lead to particle transportation, as observed in the case of fluidized beds in chemical reactors [3] and internal erosion of embankment dams and flood embankments [4,5].

Empirical and theoretical equations describe the variation in permeability, porosity, particle size, specific surface area, and pore geometry [6–8]. The commonly used Hazen equation applies to coarse soils and considers only a characteristic particle size [9]. The semi-empirical Kozeny-Carman (KC) equation was derived by assuming laminar flow conditions and applying the Hagen-Poiseuille equation to a collection of parallel cylindrical tubes [10]. The validity of the KC equation has been demonstrated through numerous experimental tests and numerical simulations [6,7,11]. The KC equation is accepted to be more accurate than the Hazen equation and can consider variations in particle size distribution [11,12], fractal pore geometry [13,14], and particle shape [15,16].

A pressure drop in fluid flow imposes a fluid-particle interaction force on the particles. Analytical expressions for these fluid-particle interaction forces were originally derived from theoretical analysis using

energy balance [17,18]. The accurate estimation of fluid-particle interactions is critical to simulate the hydro-mechanically coupled processes in granular materials [19,20]. Pore-scale flow simulations have been used widely to correlate the mean drag force with Reynolds number and solid fraction in monodisperse and polydisperse packing of spheres and validate empirical and theoretical equations [21–23]. However, the particle-to-particle variation of fluid-particle interactions cannot be characterized using these equations as they do not explicitly consider the local heterogeneities in the packing that exist in any granular material [24–26].

In comparison with assemblies of spheres, packings formed of irregular-shaped particles tend to have a more complex void topology, which influences both permeability [15,16,27–29] and fluid-particle interactions [30–32]. Previous studies have considered fluid-particle interaction forces for assemblies of ellipsoids [30,31], polyhedron particles [15], and natural particles [27,29,33]. However, understanding of the impact of particle shape on permeability and fluid-particle interactions remains incomplete for two primary reasons. Firstly, particle shape is a multi-scale feature and is typically quantified at three scales, i.e. form, roundness/angularity and roughness [34,35]. Therefore, the influence of particle shape should be considered at different scales. Second, a robust particle shape generator is needed to create 'virtual' particle shapes with prescribed multi-scale features [36,37]. Recently, three-dimensional (3D) printed irregular particles were generated by spherical harmonics (SHs) and tested with laboratory permeameters to develop a modified KC equation in which the specific surface area is more accurately estimated [38].

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This study investigates the influence of particle angularity on permeability and fluid-particle interactions in granular media with pore-scale computational fluid dynamics (CFD) simulations. We adopt a spherical harmonic-based method to randomly generate angular particles and use discrete element method (DEM) simulations to create dense packings of angular particles. The surfaces of these particles are used to define the boundaries to fluid flow in a series of CFD simulations. Flow field data from the pore-scale CFD simulations are used to quantify permeability, tortuosity, and the fluid-particle interaction forces. The detailed pore- and particle-scale results and statistical analyses characterize the interplay between packing density and particle angularity on permeability and fluid-particle interactions.

2. Angular particles generation with spherical harmonics

Spherical harmonics (SHs) are a complete set of orthogonal functions in spherical coordinates. Any function defined on a spherical surface can be written as a combination of SHs:

$$f(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^l c_l^m Y_l^m(\theta, \phi) \quad (1)$$

where $Y_l^m(\theta, \phi)$ and c_l^m are the SH and the SH coefficient at degree l and order m , $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi]$ are the latitudinal and longitudinal coordinates. SHs have been widely adopted to reconstruct irregular particle shapes by decomposing the radius $r(\theta, \phi)$ into spherical coordinates [39–41]. However, this reconstruction is limited to 'star-like' particles since all the particle surface vertices have to be uniquely represented with spherical coordinate.

SHs expansions can also reconstruct a three-dimensional particle surface in Cartesian coordinates after surface parametrization [42,43]:

$$\mathbf{v}(\theta, \phi) = \begin{bmatrix} x(\theta, \phi) \\ y(\theta, \phi) \\ z(\theta, \phi) \end{bmatrix} = \begin{bmatrix} \sum_{l=0}^{\infty} \sum_{m=-l}^l c_{x,l}^m Y_l^m(\theta, \phi) \\ \sum_{l=0}^{\infty} \sum_{m=-l}^l c_{y,l}^m Y_l^m(\theta, \phi) \\ \sum_{l=0}^{\infty} \sum_{m=-l}^l c_{z,l}^m Y_l^m(\theta, \phi) \end{bmatrix} \quad (2)$$

The Cartesian SH decomposition requires more SH coefficients than that in spherical coordinates and has two major advantages: (a) any closed 3D surface can be reconstructed, including non-star-like shapes; and (b) multi-scale shape parameters can be derived directly from SH coefficients.

Zhao et al. [44] proposed two shape descriptors directly defined from SH coefficients in Cartesian coordinates to quantify particle form and roundness, respectively. Particle form is quantified using the principal dimensions of the ellipsoid defined by the first-degree SHs, while angularity is quantified using the relative importance of surface features defined with SH degrees between 2 and 8. Specifically, particle angularity is defined as $D_{2-8} = d_{2-8}/d_1$, where d_l is the spherical descriptor at degree l :

$$d_l = \sqrt{\sum_{i \in \{x, y, z\}} \sum_{m=-l}^l \|c_{i,l}^m\|^2} \quad (3)$$

Image processing methods have also been developed to quantify 3D particle shapes at different scales (e.g., [35]). Zhao et al. [44] showed that the SH-based angularity agrees well with the more traditional particle angularity measure determined by local surface curvatures for angular sand particles and their fragments.

An irregular particle shape generator based on Spherical Harmonics was proposed by Wei et al. [37] to randomly construct SH coefficients and generate an unlimited number of 'virtual' particles with

pre-defined multi-scale shape parameters, e.g. form, roundness and roughness. The method mainly involves two steps: (a) an ellipsoid corresponding to the first-degree SHs is generated with specified aspect ratios, i.e. the ratios between three principal dimensions; and (b) the SH coefficients of degrees two to eight are randomly constructed from a specified D_{2-8} angularity. In addition, smaller surface textures (e.g., roughness) can also be randomly constructed with the SHs degree higher than eight.

We used the Spherical Harmonics Particle Shape Generator (SHPSG) code, which was implemented in Python to generate the STL files for irregular shapes [45]. The first-degree SH coefficients correspond to a sphere to avoid the influence of particle form. Particles with different levels of angularity were generated with D_{2-8} values of 0.1, 0.2, 0.3, 0.4, and 0.5; Zhao et al. [44] found that the D_{2-8} angularity level of angular sand particles and their fragments was between 0.2 and 0.5. One thousand particles were randomly generated for each angularity level, and for each angularity level two typical particles are shown in Fig. 1a. The virtual particles generated using these parameters have an averaged aspect ratio larger than 0.9 and a curvature-based roundness value between 0.5 and 0.9 [37].

3. Gravity deposition of irregular-shaped particles in DEM

3.1. Overlapping sphere construction

DEM simulations of gravity deposition were carried out to construct dense granular packings, where each non-spherical particle was represented as a clump of overlapping spheres. The efficiency of this method depends mainly on the overlapping spheres construction method, in which the position and radius of spheres are determined within the irregular particle surface. Many algorithms have been proposed to generate overlapping spheres [46–48]. However, these algorithms may lead to an unnecessarily large number of spheres or suffer from a high computational cost. Therefore, this study adopted a new, simple method to generate overlapping spheres for any irregular shape using image processing and an optimization algorithm. Fig. 1b shows the constructed thirty overlapping spheres for two typical particles with each angularity level.

To create a sphere clump, the surface of a particle generated with the SHPSG was voxelized into a three-dimensional binary image with 50 pixels along each dimension. A higher number of pixels will slightly increase the accuracy with which the particle surface topology is captured but reduce the speed of optimization. We then calculated the 3D distance map of the binary image with the Euclidian distance transform (Fig. 2a). The value of each pixel on a distance map indicates the radius of the maximum inscribed sphere centred at that pixel. Incorporating this image processing stage reduces dramatically the calculation cost associated with finding the radius of the maximum inscribed sphere centred at a given pixel.

The third step is to identify a series of spheres to fill the particle surface. The centre of the first optimum sphere coincides with the pixel having the maximum value in the distance map (Fig. 2b). An optimization algorithm is required to find the centres of the subsequent optimum spheres. This study adopted the differential evolution algorithm for optimization [49]. The objective function is the filling ratio, R_f , which is defined as the ratio between the filled volume and the total particle volume. The parameters for optimization are the coordinates of each sphere centre. The distance map was used to determine the radius of the maximum inscribed sphere for the potentially optimal spheres. Then their corresponding filled region was used to update the filling ratio R_f . Fig. 2 b-d show the unfilled region in black for a typical angular particle where the number of overlapping spheres (N_{sph}) is 1, 3 and 30, respectively.

The filling ratio initially increases rapidly with N_{sph} and approaches a value of one asymptotically at large N_{sph} values, as shown in Fig. 3. For a given N_{sph} , more angular particles with a higher D_{2-8} have a lower R_f

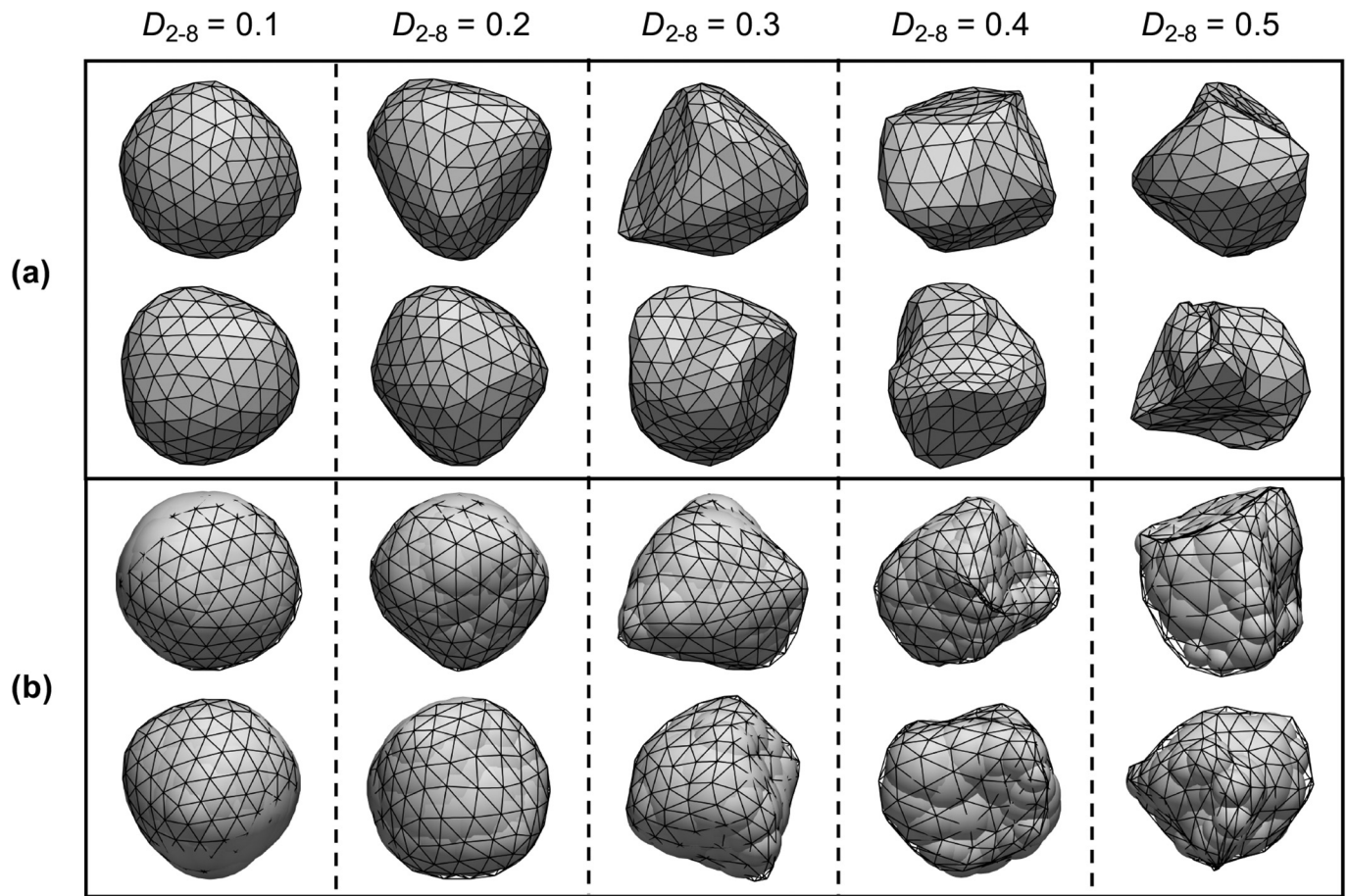


Fig. 1. Irregular particle shapes randomly generated by the Spherical Harmonics Particle Shape Generator (SHPSG) with different levels of angularity $D_{2-8} = [0.1, 0.2, 0.3, 0.4, 0.5]$. For each D_{2-8} value, two typical particles are shown as (a) particle surfaces and (b) particles filled with overlapping spheres.

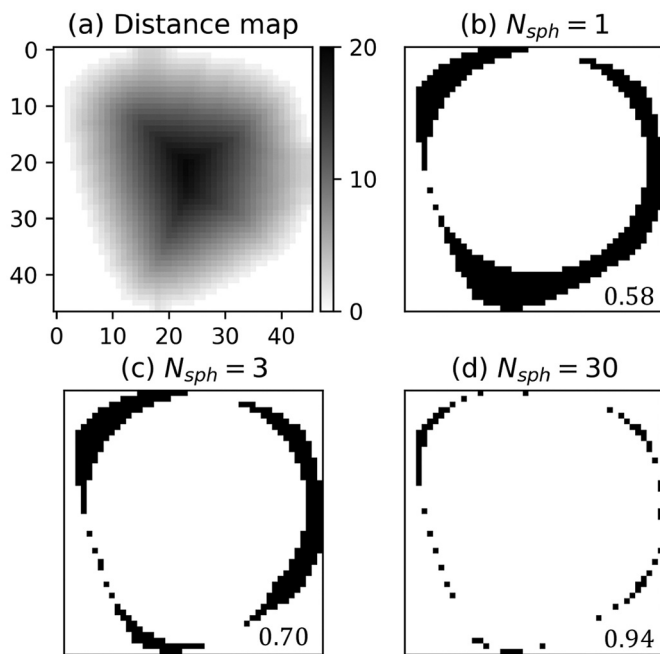


Fig. 2. Two-dimensional illustration of overlapping sphere construction method for a particle with $D_{2-8} = 0.4$: (a) distance map (dimension in pixels); (b-d) the unfilled region is illustrated in black for different numbers of overlapping spheres (N_{sph}). Filling ratios are shown at the lower right corner for (b-d).

due to the difficulty in filling the sharp corners of angular particles (see Fig. 1b, $D_{2-8} = 0.5$). We selected thirty overlapping spheres for each particle since the rate of increase in R_f with increasing N_{sph} is very small for $N_{sph} > 30$. Achieving a filling ratio of one was not a requirement for the CFD analyses considered here. Fig. 4 shows the distribution of R_f values for one thousand particles for each angularity level

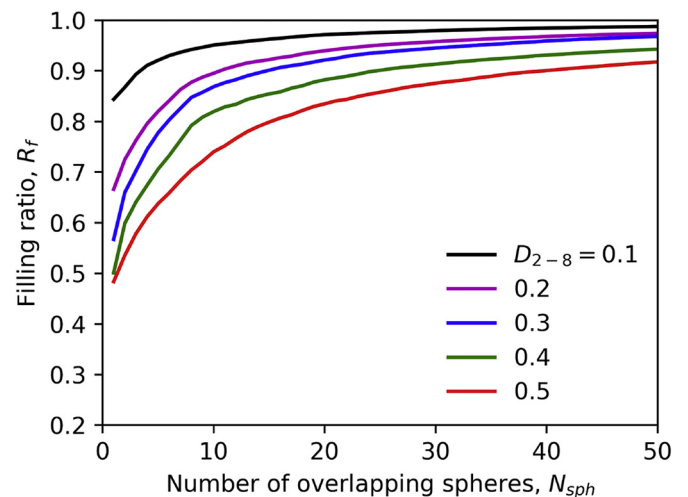


Fig. 3. Increase in filling ratio with the number of overlapping spheres for five typical particles with different levels of angularity.

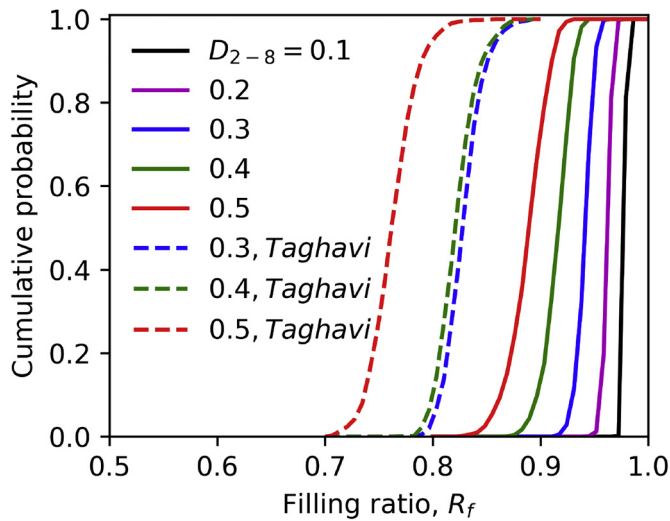


Fig. 4. Cumulative distributions of filling ratios for one thousand particles randomly generated for each angularity level. Thirty overlapping spheres are used to fill each particle. Dashed lines indicate the filling ratios with about 100 overlapping spheres generated by the bubble packing algorithm [40] available in PFC v5.0 [22].

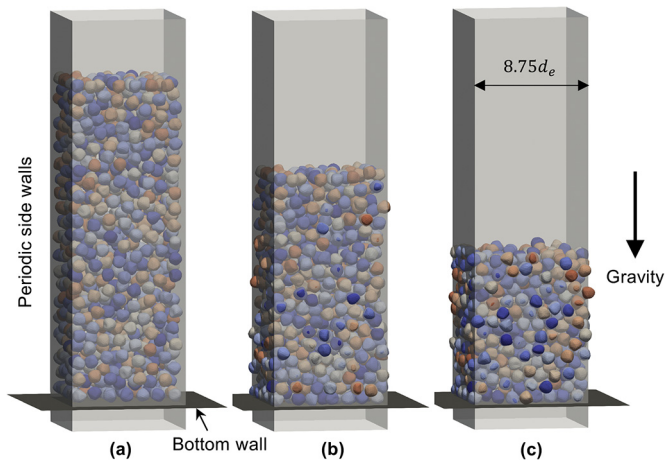


Fig. 5. Gravity deposition process to construct the initial dense packing for the sample with $D_{2-8} = 0.2$: (a) initial state; (b) during deposition; (c) after deposition.

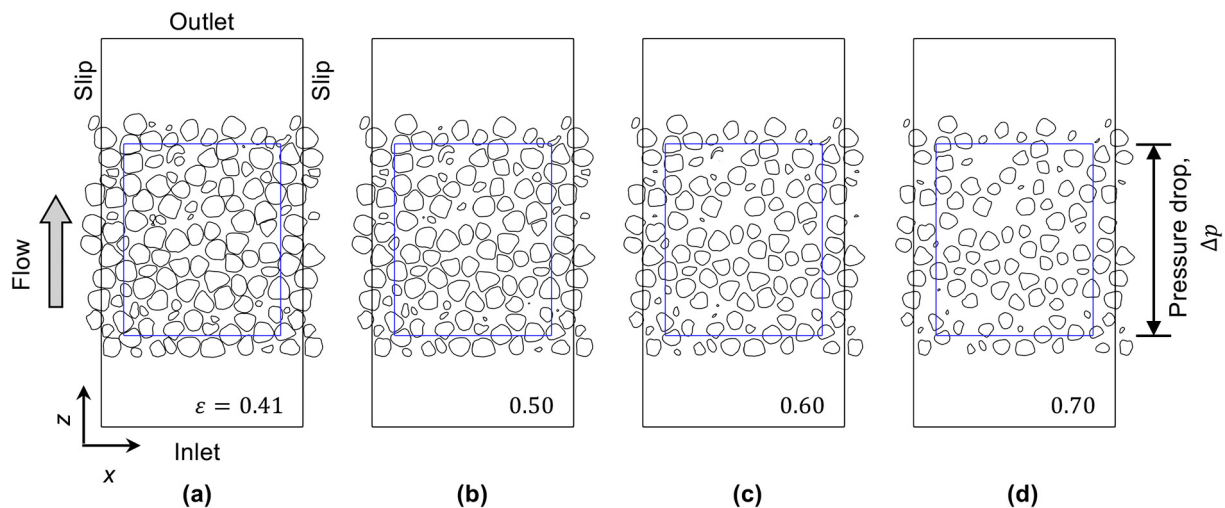


Fig. 6. Vertical cross-sectional images of samples with angularity $D_{2-8} = 0.3$ and various porosity values (a–d). The boundary conditions of CFD models are labeled for the sample with porosity $\varepsilon = 0.41$ (a). Only particles completely inside the blue rectangular are used for fluid-particle interaction analysis. Permeability is estimated by the pressure drop within the blue rectangle.

considered with $N_{sph} = 30$. The filling ratio is larger than 0.9 for most particles with $D_{2-8} \leq 0.4$. The most angular particles with $D_{2-8} = 0.5$ have a $R_f \in [0.85, 0.92]$. To test the efficacy of this new method, the overlapping spheres for 1000 particles with $D_{2-8} = 0.3, 0.4$ and 0.5 were generated using the bubble packing algorithm proposed by Taghavi [48] which is available in PFC3D v5.0 [50]. Each particle was filled with about 100 overlapping spheres. The distributions of filling ratio were shown as dashed lines in Fig. 4. The new method proposed in this study leads to about 10% higher filling ratio with about 70% less overlapping spheres than Taghavi's bubble packing algorithm. The smaller number of spheres will measurably reduce the calculation cost for DEM simulations of irregular-shaped particles.

3.2. Gravity deposition in DEM

This study used DEM to construct a random dense packing of irregular particles. The positions of the particles remained fixed during the CFD simulations, i.e. the data were not generated using coupled CFD-DEM simulations. The DEM simulations were performed with the open-source discrete element code, YADE [51]. In all cases, dense packing of 1000 spheres with a diameter of 2 mm was firstly generated and subjected to isotropic compression of 1 kPa. The height of the compression box was about two times its width, so that the sample was initially tall. The spheres were then replaced by angular particles with a smaller equivalent spherical diameter $d_e = 1.6$ mm (Fig. 5a). The smaller particle size ensures that the replaced particles do not overlap with each other. Then, the overlapping spheres generated for each irregular particle were imported as a clump, which behaves as a rigid body. The clump's mass and inertia tensor were estimated after converting a clump into cells with regular grid spacing in YADE. This step avoids incorrect mass and moment of inertia, which are important for the kinematics of irregular particles [46].

As illustrated in Fig. 5, a vertical body force was activated to enable the particles to migrate downwards into a dense packing. The simulations adopted density, Young's modulus and Poisson's ratio values typical of quartz sand [52]. The friction ratio at the contacts was set to be zero to obtain a high packing density. Periodic boundaries were used at four vertical walls; this avoids the large voids usually encountered between sidewalls and particles. The porosity of the samples following gravity deposition was between 0.40 and 0.41. After gravity deposition, the STL surfaces were updated using the translation and rotation of each clump. The size of all particles was scaled (reduced) in a controlled manner to achieve four values of packing porosity $\varepsilon = 0.41, 0.5, 0.6$

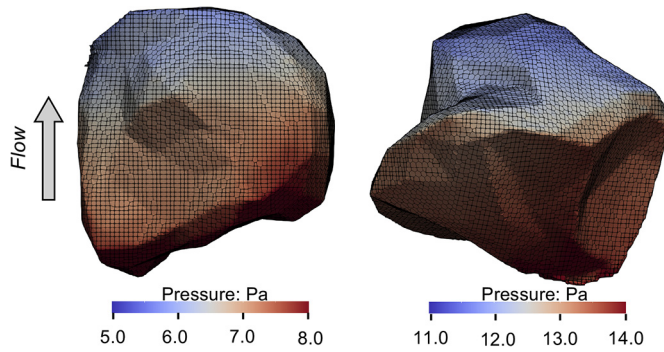


Fig. 7. Surface mesh of two particles with $D_{2-5} = 0.5$ in CFD model and the resulted pressure distributions.

and 0.7 (Fig. 6a-d). The particle centroids remained unchanged as the particle size was reduced. Finally, one thousand irregular particles together with the ghost particles at periodic boundaries were combined into a single STL file representing the packing geometry.

4. Computational fluid dynamics (CFD) simulations

4.1. CFD model

This study used computational fluid dynamics (CFD) simulations to solve the incompressible Navier-Stokes equation in the pore space defined by the irregular particle packings with the open-source CFD toolbox OpenFOAM [53]. The Semi-Implicit Method of Pressure Linked Equations, or SIMPLE algorithm, was adopted to simulate steady-state laminar flow. The Reynolds number, Re , was confirmed to be less than 0.1 in all cases as calculated using the following equation

$$Re = \frac{\rho v d_e}{\mu} \quad (4)$$

where ρ is the fluid density, μ is the dynamic viscosity, and v is the superficial flow velocity. The fluid had a dynamic viscosity of $0.001 \text{ Pa} \cdot \text{s}$ and a density of 1 g/cm^3 . Fig. 6a shows the boundary conditions in the CFD models. A constant velocity of 0.02 mm/s and a constant pressure of 0 Pa were applied at the inlet and outlet, respectively. ‘Slip’ boundaries were applied at four sidewalls so that the velocity component normal to each wall is set to zero while the tangential velocities remain unconstrained. ‘No-slip’ boundaries were applied to all particle surfaces

so that the velocities normal and tangential to surface were constrained to be zero.

The CFD domain was discretized by a mesh generation algorithm in OpenFOAM, i.e., SnappyHexMesh. This algorithm trims regular blocks with the STL file of granular packings. Local refinement was adopted to resolve the narrow channels between neighbouring particles, especially for dense packings. The resultant mesh has around 60 million elements. The typical computation time is about 1.5 hrs for a parallel computing with 64 cores on a high performance computing cluster (HPC). The average particle to mesh size ratio was around 40. The sharp corners of angular particles are well resolved with SnappyHexMesh at the current mesh size (Fig. 7). The CFD analysis provided the velocity and pressure values at the centre of each CFD cell.

The normal and shear stresses on the particle surfaces were determined from the velocity and pressure fields in the fluid. Then, the normal pressure and viscous shear stress over all surface elements on each particle were integrated to obtain the pressure component ($\mathbf{F}_p$) and viscous component ($\mathbf{F}_v$) of the fluid-particle interaction force ($\mathbf{F}_{f-s}$) on an individual particle:

$$\mathbf{F}_p = \sum_i \rho p_i A_i \mathbf{n}_i \quad (5)$$

$$\mathbf{F}_v = \sum_i \mu \mathbf{R}_{dev,i} A_i \quad (6)$$

$$\mathbf{F}_{f-s} = \mathbf{F}_p + \mathbf{F}_v \quad (7)$$

where ρ is the fluid density, and μ is the dynamic viscosity; for the i^{th} surface element, p_i is the normal kinematic pressure, A_i and $\mathbf{n}_i$ are the triangular element area and normal vector, and $\mathbf{R}_{dev,i}$ is the deviatoric stress tensor. The integral was performed using the built-in function ‘forces’ in OpenFOAM. Referring to Fig. 6, a blue rectangle was defined with a distance of d_e from sidewalls or packing boundaries. Each sample had about 300 particles that are completely within the blue rectangle, and these particles were used for the fluid-particle interaction analyses.

4.2. Validation of fluid-particle interactions

The fluid-particle interaction forces estimated from the CFD analyses were validated with the numerical solutions from Zick & Homsy [54] for simple cubic (SC) and face-centred cubic (FCC) packings of uniformly sized spheres. The validation models exploited geometric symmetry to reduce the calculation cost. Fig. 8a shows the FCC simulation setup.

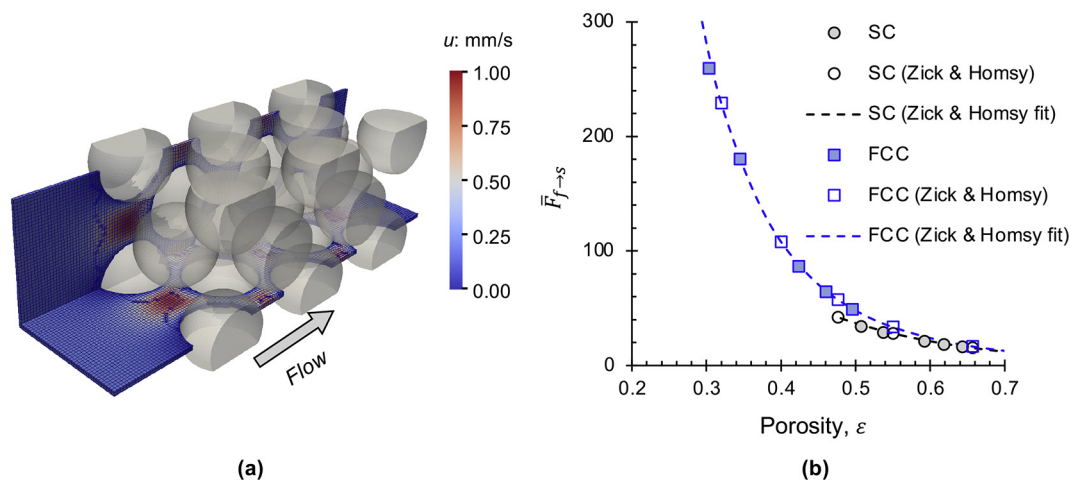


Fig. 8. (a) Simulation setup for FCC model with periodic boundaries parallel to the flow direction. Mesh size and velocity field are indicated. Inlet velocity is 0.2 mm/s . (b) Validation of fluid-particle interactions for SC and FCC packings. The results from Zick & Homsy [57] and their fitting curves are included.

The boundary conditions are identical to the permeameter models, except for the 'cyclic' boundary conditions applied to the four sidewalls. The sphere centroids were placed on a fixed lattice, and the particle diameters were controlled to reach different packing densities. The fluid-particle interaction coefficient, $\bar{F}_{f \rightarrow s}$, is defined as the fluid-particle interaction force normalized by Stokes drag force $F_{f \rightarrow s}^s$ in the z-direction:

$$F_{f \rightarrow s}^s = 3\pi\mu d v \quad (8)$$

$$\bar{F}_{f \rightarrow s} = \frac{|\mathbf{F}_{f \rightarrow s}|}{F_{f \rightarrow s}^s} = \frac{|\mathbf{F}_p + \mathbf{F}_v|}{F_{f \rightarrow s}^s} \quad (9)$$

where d is the particle diameter, v is the superficial flow velocity. The fluid-particle interaction coefficients estimated from CFD models were in good agreement with the Zick & Homsy solutions at different packing forms and densities, as shown in Fig. 8b [55].

5. Results

5.1. Permeability estimation

The permeability was estimated from the pressure drop Δp within the blue rectangular area, as shown in Fig. 6d. Fig. 9a compares the estimated normalized permeability k/d_e^2 with values obtained using the Kozeny-Carman (KC) equation. According to the KC equation, permeability can be predicted from

$$k_{KC} = \frac{1}{C_{KC}} \cdot \frac{1}{S_0^2} \cdot \frac{\varepsilon^3}{(1-\varepsilon)^2} \quad (10)$$

where C_{KC} is the Kozeny-Carman empirical coefficient, typically $C_{KC}=5$; S_0 is the specific surface of particles, which equals to $6/d$ for spheres [6]. Therefore, the equation becomes

$$\frac{k_{KC}}{d^2} = \frac{\varepsilon^3}{180(1-\varepsilon)^2} \quad (11)$$

The KC equation predicts the permeability for the dense packings and highly overestimates the permeability for diluted systems for the $D_{2-8} = 0.1$ samples with almost spherical particles.

Zick & Homsy [57] provided the fluid-particle interaction coefficients, $\bar{F}_{f \rightarrow s}$, for a series of porosity levels for FCC packings. We adopted

spline interpolation to fit a relationship between $\bar{F}_{f \rightarrow s}$ and porosity. Then, the permeability values can be estimated from $\bar{F}_{f \rightarrow s}$ through

$$\frac{k_{ZH}}{d^2} = \frac{1}{18(1-\varepsilon)\bar{F}_{f \rightarrow s}} \quad (12)$$

Fig. 9a shows that the Zick & Homsy solutions agree better with the permeability data from our CFD analyses than the KC equation for dilute packings.

The packings with more angular particles tend to have a lower permeability (Fig. 9). For example, about 30% reduction in permeability occurs as D_{2-8} increases from 0.1 to 0.5 in the densest packing. The influence of particle angularity can be partially reflected by the evolving specific surface, where the averaged $1/S_0^2$ reduces by about 23% if D_{2-8} changes from 0.1 to 0.5. This demonstrates the ability of the KC equation to predict the influence of particle shape on permeability to some extent. Interestingly, the influence of particle angularity seems to be porosity-dependent. The reduction of permeability when D_{2-8} increases is less significant for the dilute cases when the influence of particle angularity on flow fields becomes less important (Fig. 9b).

5.2. Tortuosity

The influence of pore heterogeneity on permeability is commonly attributed to the flow tortuosity, which quantifies the curvature of flow streamlines. This study adopted the method proposed by Duda et al. [56] to determine tortuosity with flow fields instead of randomly selected streamlines:

$$T = \frac{\langle |\mathbf{u}| \rangle}{\langle u_z \rangle} \quad (13)$$

where $\langle |\mathbf{u}| \rangle$ and $\langle u_z \rangle$ are the mean magnitude of flow velocity vector and the mean z-direction component of flow velocity vector parallel to the macroscopic flow direction, respectively. The tortuosity is always larger than one and increases as the relative importance of the parallel flow component reduces. We selected seven vertical slices located at $y = 6, 8, 10, 12, 14, 16$, and 18 mm, and quantified the averaged tortuosity with their velocity fields.

As shown in Fig. 10, the relationship between tortuosity and porosity could be described well with an exponential equation:

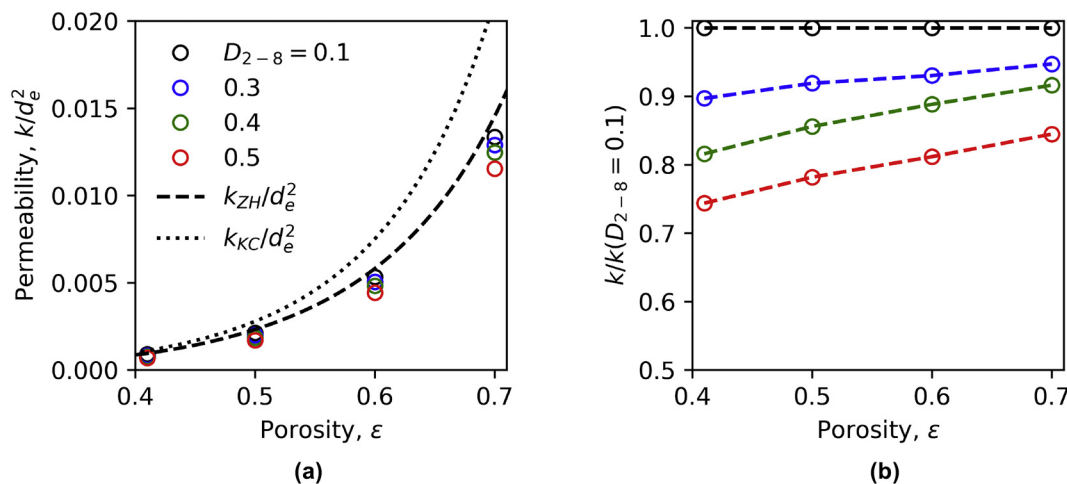


Fig. 9. (a) Influence of porosity and angularity on the permeability estimated by CFD models. Dashed line indicates the permeability estimated by Kozeny-Carman (KC) equation and the fitted Zick & Homsy (ZH) solutions. (b) Permeability reduction ratio as angularity increases from $D_{2-8} = 0.1$.

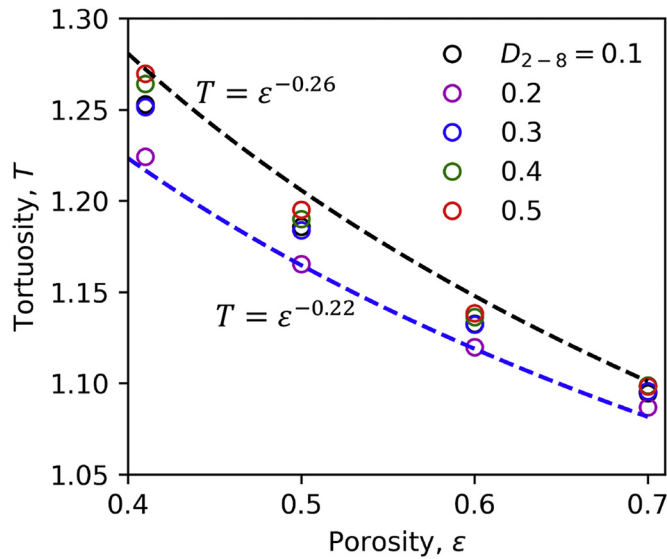


Fig. 10. Influence of packing porosity and particle angularity on flow tortuosity.

$$T = \varepsilon^{-q} \quad (14)$$

where q varies from 0.22 to 0.26. However, the influence of angularity on tortuosity is not obvious. For example, the packings of particles with $D_{2-8} = 0.2$ have the smallest tortuosity in each porosity level, although $D_{2-8} = 0.5$ samples have the highest tortuosity. This non-monotonic dependence of T on D_{2-8} indicates that the relative positions between particles are more important than particle angularity in determining flow tortuosity since particle angularity only influences flow fields locally. The variation in tortuosity with angularity will differ if the packing configuration differs. The packing configurations for each angularity in this study depends on the DEM simulation used to generate the densest samples. Therefore, the tortuosity of samples with five angularity levels in each porosity level follows a consistent order since the relative position between particles remains unchanged.

5.3. Flow fields

Fig. 11 shows the typical distributions of horizontal and vertical components of flow velocity vector on the x - z plane at the middle of

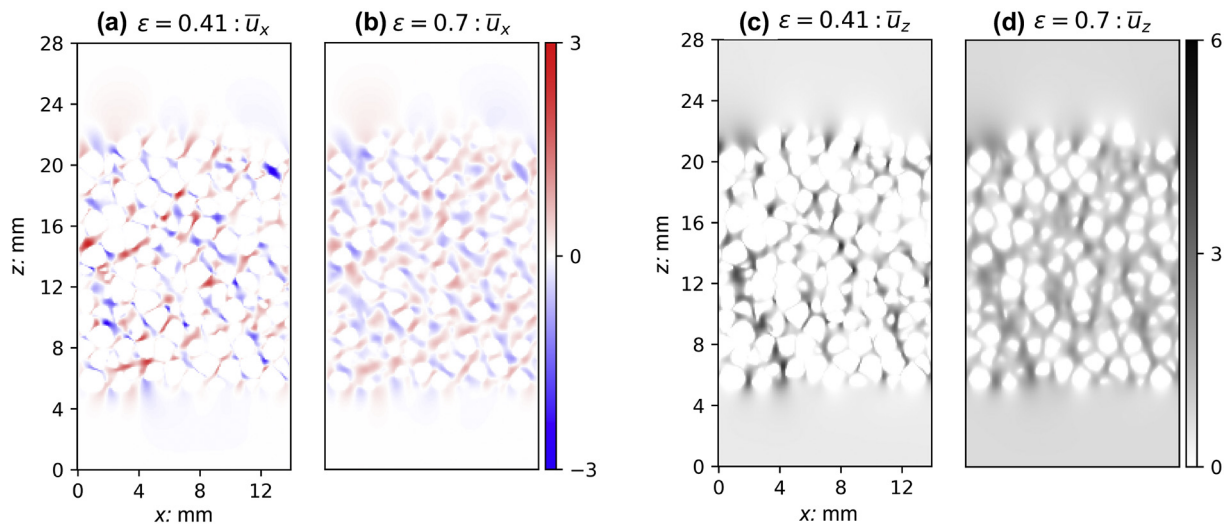


Fig. 11. Distributions of normalized horizontal velocity (a-b) and vertical velocity (c-d) in two samples with different porosities and $D_{2-8} = 0.4$. Velocity is normalized by the seepage velocity.

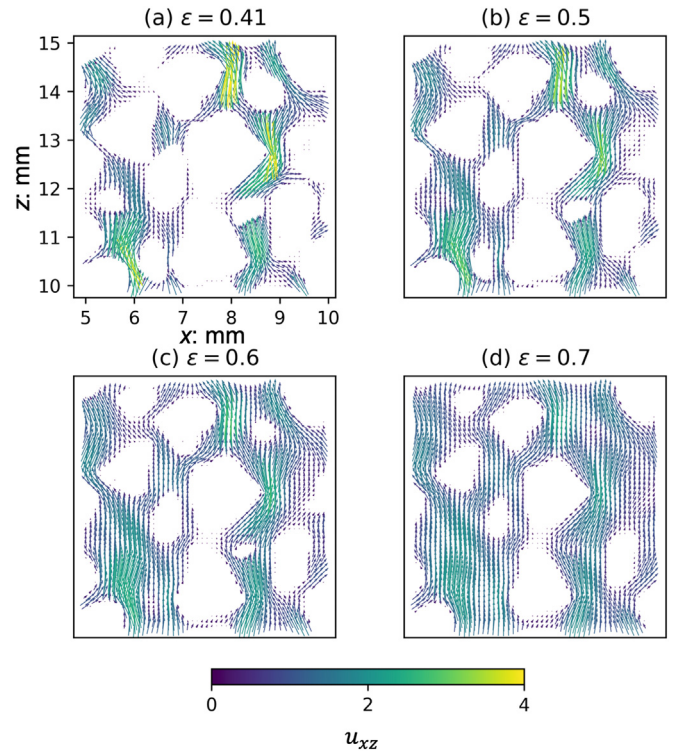


Fig. 12. Influence of porosity on the vector plots of flow fields for the samples with $D_{2-8} = 0.4$.

the samples for two porosities in the case of particles with angularity $D_{2-8} = 0.4$. The flow velocity components $\bar{u}_x$ and $\bar{u}_z$ are normalized by the seepage velocity, which is the superficial velocity divided by porosity. The flow fields are very uniform in the dilute samples. As the porosity reduces, the flow fields become more heterogeneous, and a few large pores emerge as part of the preferential flow paths, where flow rates are much higher. The horizontal flow is prohibited at two sidewalls where $\bar{u}_x = 0$. According to Fig. 11 a & b, the influence of this boundary effect is limited to a small region.

The vector plots of flow fields are shown for a smaller region of about $5 \times 5 \text{ mm}^2$ to further illustrate the influence of packing density and particle angularity (Figs. 12–13). As porosity increases from 0.41 to 0.7, the

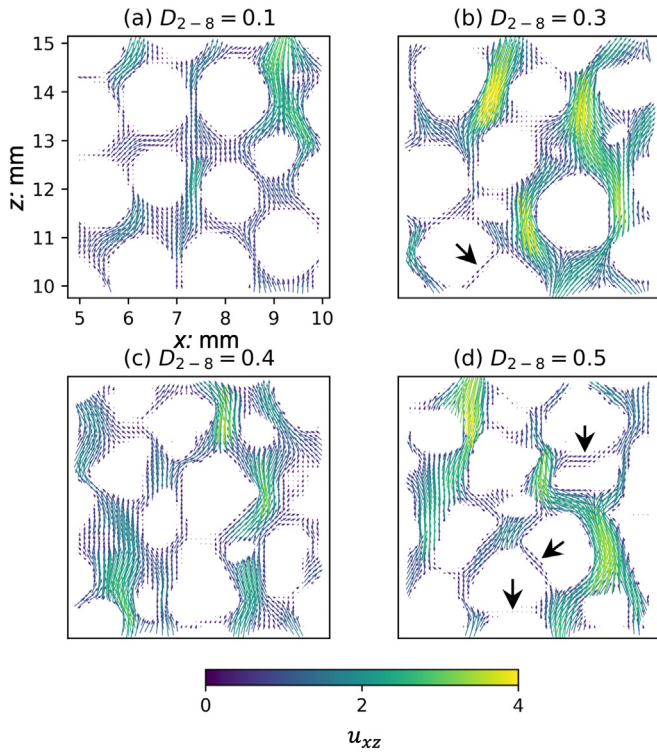


Fig. 13. Influence of angularity on the vector plots of flow fields for the samples with porosity $\varepsilon = 0.5$. Arrows indicate straight channels between particles.

flow field becomes more uniform, and the maximum normalized flow rate reduces (Fig. 12). The locations of the fast-flow regions remain almost unchanged as the packing density changes. This is mainly because the relative positions and the orientation of particles are fixed as porosity changes. Fig. 13 shows the influence of angularity on the flow vector plot at a packing porosity $\varepsilon = 0.5$. For spherical particles, the flow channels appear to have mostly converging-diverging patterns. However, narrow straight channels can form between the flat surfaces of angular particles, as highlighted by the black arrows.

Fig. 14 shows the normalized flow rate distributions on the middle vertical plane within the sample. The normalized vertical flow rate becomes more concentrated around one as packing porosity increases, while the horizontal flow rate becomes smaller. A similar influence of packing density on flow rate distributions was reported in Rong et al., (2013). Particle angularity has limited impacts on the flow rate distributions for both dense and dilute packings, as shown by Fig. 15. This further demonstrates that the influence of particle angularity is localized.

5.4. Fluid-particle interactions

The vector plots of fluid-particle interaction forces in Fig. 16a show the variance in the magnitude and direction within a monodisperse sample. The fluid-particle interaction coefficient data tend to follow a normal distribution (Fig. 16b). Most of the fluid-particle interaction coefficient values are between 17 and 35, with a relative difference of around 100%. The directions of the fluid-particle interaction forces have a small deviation from the macroscopic flow direction. Fig. 17a shows that no clear relationship exists between the horizontal fluid-particle interaction force, $\bar{F}_{f \rightarrow s, xy}$, and the vertical fluid-particle

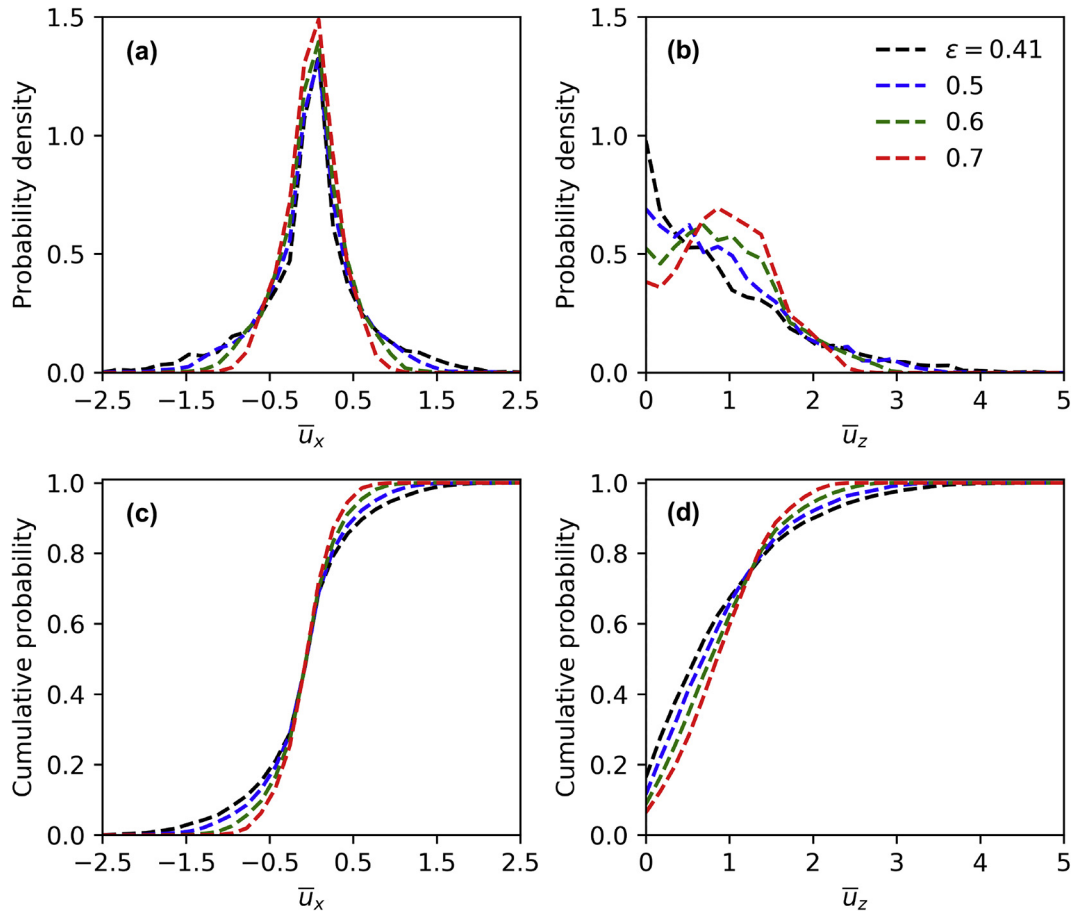


Fig. 14. Influence of porosity on the density and cumulative distributions of normalized horizontal and vertical flow velocity for the samples with $D_{2-8} = 0.4$.

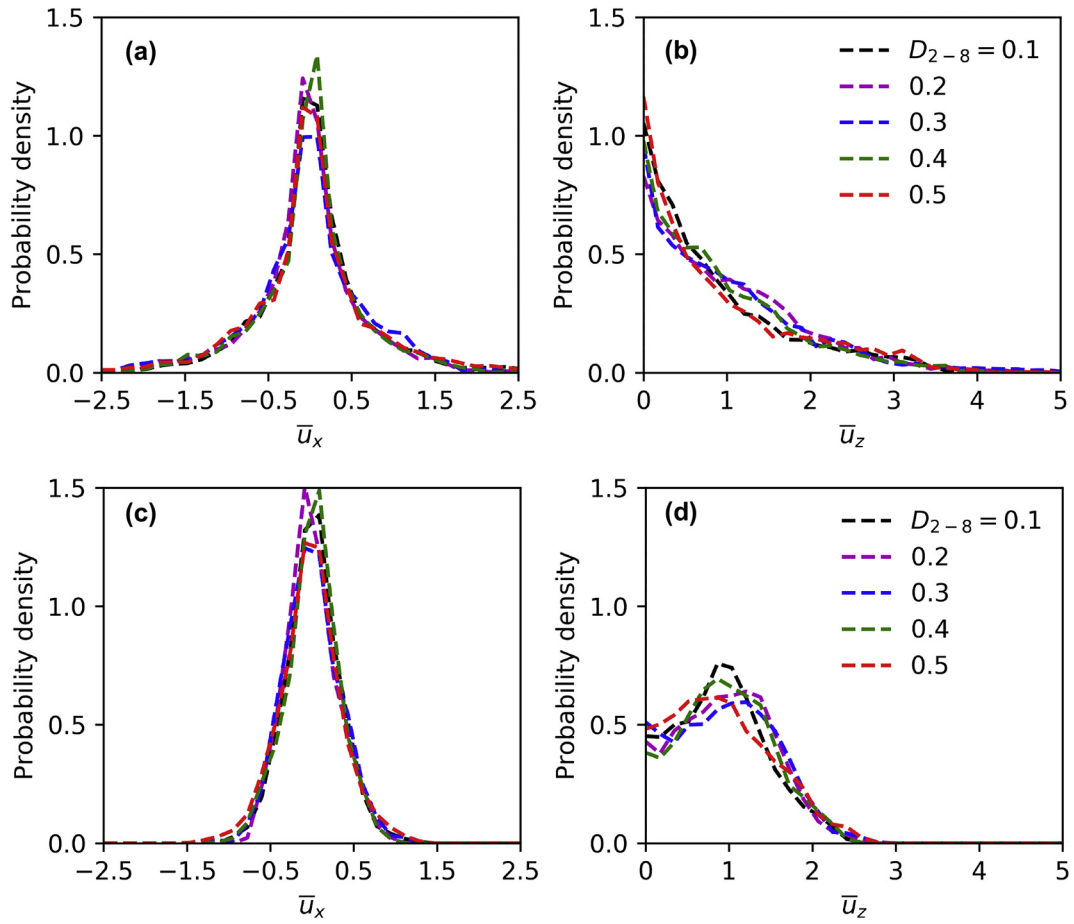


Fig. 15. Influence of angularity on the density distributions of flow velocity along x and z in the samples with porosity $\varepsilon = 0.41$ (a-b) and $\varepsilon = 0.7$ (c-d).

interaction force, $\bar{F}_{f \rightarrow s, z}$. The ratio of the mean values of $\bar{F}_{f \rightarrow s, xy}$ and $\bar{F}_{f \rightarrow s, z}$ gives a deviation angle from the macroscopic flow direction of $\theta_d = \arctan(3.3/25.4) = 12^\circ$. The viscous and pressure components of the fluid-particle interaction forces tend to form a linear relationship (Fig. 17b). In this particular sample, the mean ratio between the viscous

and pressure components is about 0.5, and most data are within $\pm 20\%$ of this linear relationship.

Fig. 18a shows that the mean value of fluid-particle interaction coefficients in each sample reduces as the porosity increases. This relationship for $D_{2-8} = 0.1$ is well predicted by the solutions for FCC packings

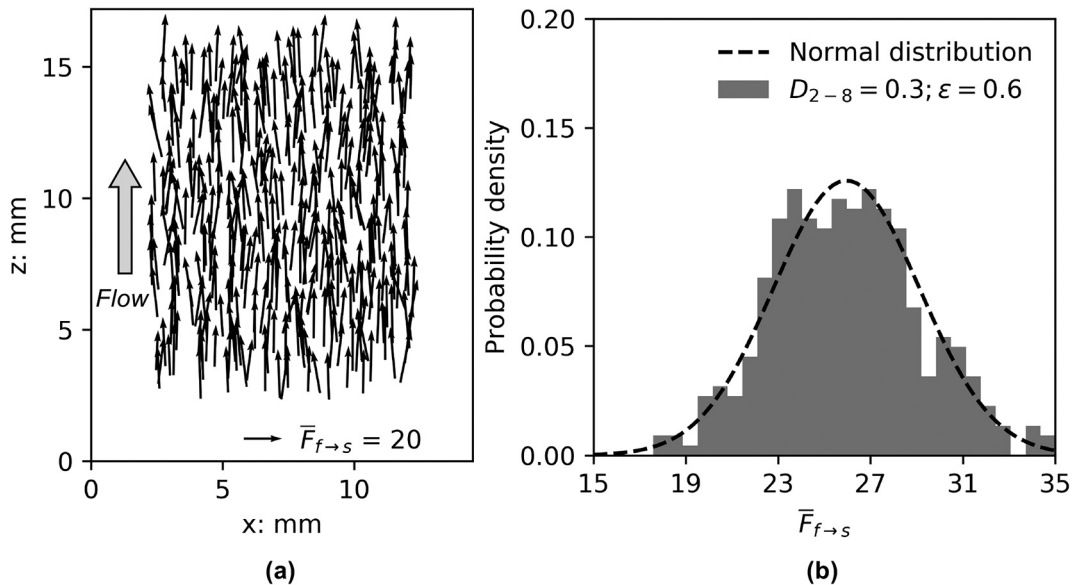


Fig. 16. (a) Projection of normalized fluid-particle interaction forces on x-z plane. (b) Distribution of fluid-particle interaction coefficients and the fitted normal distribution. The sample considered has $D_{2-8} = 0.3$ and $\varepsilon = 0.6$.

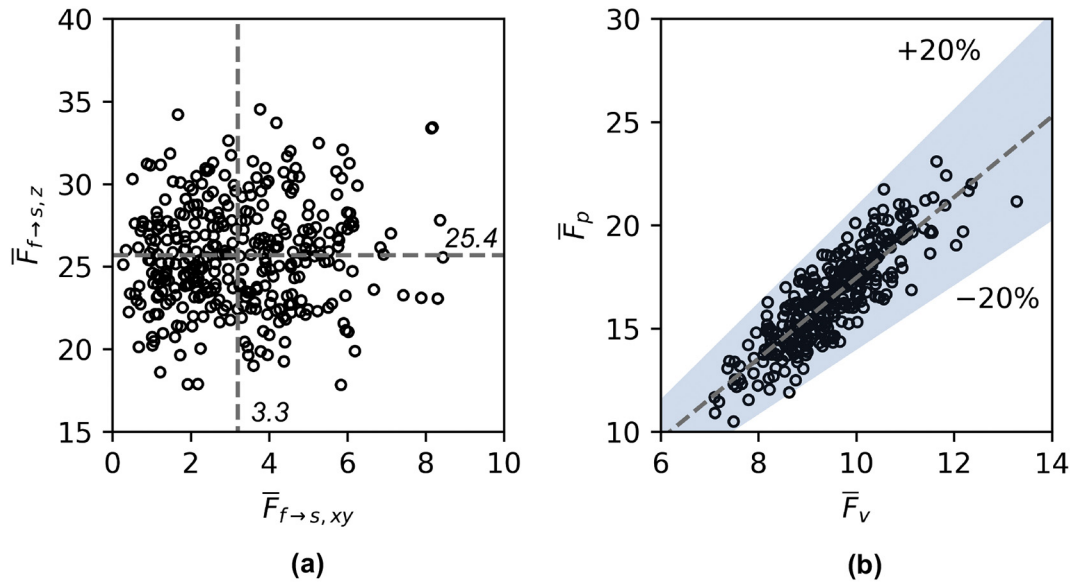


Fig. 17. (a) Comparison of horizontal and vertical components of fluid-particle interactions. (b) Comparison of viscous and pressure components of fluid-particle interactions. The sample has $D_{2-8} = 0.3$ and $\varepsilon = 0.6$.

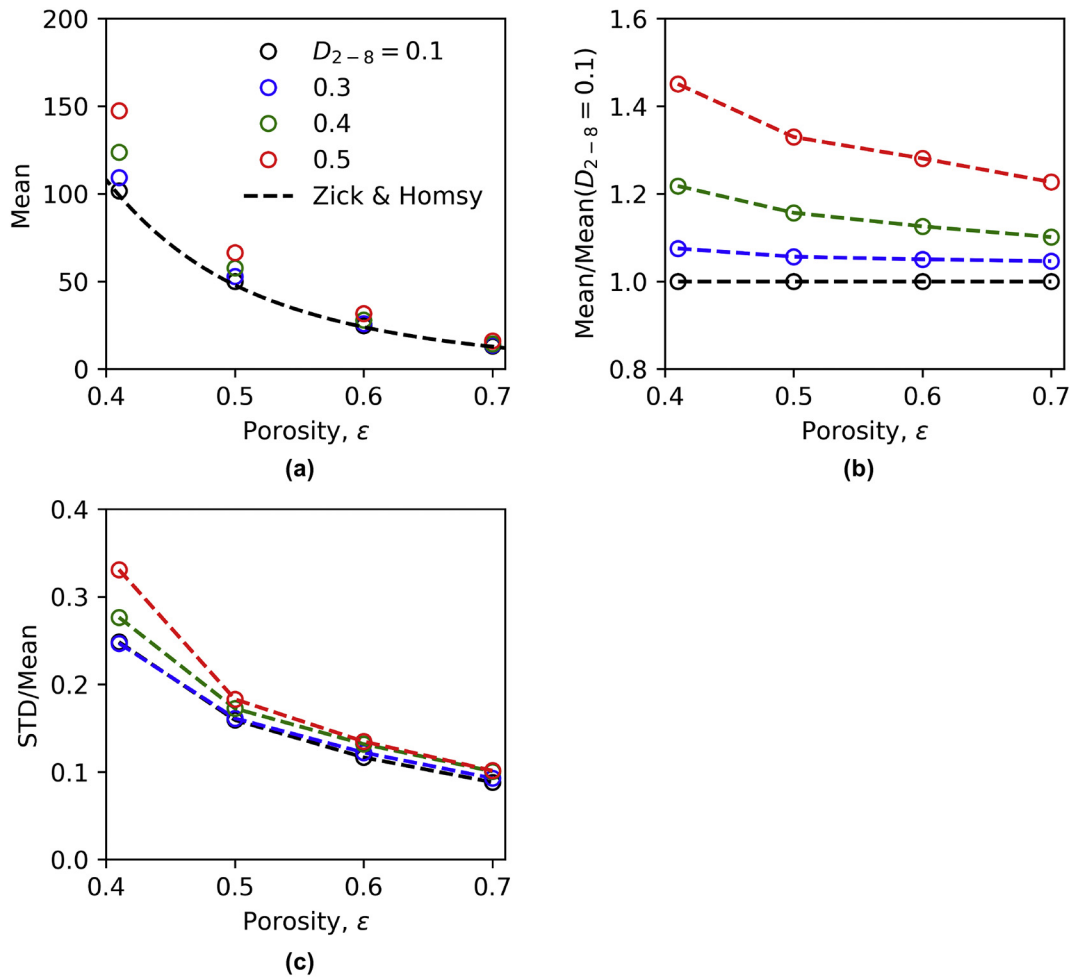


Fig. 18. Influence of porosity and angularity on fluid-particle interaction coefficients: (a) mean value in each sample; (b) mean value normalized by the sample with $D_{2-8} = 0.1$; (c) normalized standard deviation (STD/Mean).

of spheres from Zick & Homsy [57]. The packings with more angular particles tend to have higher mean fluid-particle interaction coefficients. As shown in Fig. 18b, $\bar{F}_{f \rightarrow s}$ increases by 45% and 23% as the angularity D_{2-8} increases from 0.1 to 0.5 for the densest and loosest packings, respectively. This influence is consistent with the angularity impact on permeability shown in Fig. 9. The normalized standard deviation (STD) of the fluid-particle interaction coefficients also increases with packing density and angularity, which leads to a larger variance in the fluid-particle interactions (Fig. 18c).

Fig. 19 shows the distributions of the fluid-particle interaction coefficients normalized by their mean value for each sample, $\bar{F}_{f \rightarrow s} / \langle \bar{F}_{f \rightarrow s} \rangle$. As the porosity increases, the distribution of normalized fluid-particle interaction coefficients becomes narrower. Most $\bar{F}_{f \rightarrow s} / \langle \bar{F}_{f \rightarrow s} \rangle$ values fall within $\pm 20\%$ and $\pm 60\%$ of the mean value for $\varepsilon = 0.7$ and 0.41, respectively. At each density level, angularity has a limited influence on the distributions of normalized fluid-particle interaction force.

Fig. 20 shows the distributions of the angle between the fluid-particle interaction force and the flow direction, θ_d . In the loosest case $\varepsilon = 0.7$, the distribution has a peak value at 3° and a right tail that extends to about 15° . Only a small number of particles have a fluid-particle interaction force that is colinear with the flow direction, i.e. $\theta_d = 0$. As the packing porosity reduces, the distribution becomes flatter and shifts to the right with a higher peak angle and longer right tail, which means that the horizontal fluid-particle interaction becomes more relevant. Again, angularity has a limited influence on the angle of deviation.

Fig. 21 shows the distributions of the ratio between the viscous and pressure components of fluid-particle interaction forces, $\bar{F}_v / \bar{F}_p$. In the

loosest packing $\varepsilon = 0.7$, the viscous drag is about 80% of the pressure drag component on average, while this value declines to about 20% for the densest packing. The relative importance of the viscous component increases with increasing porosity or reducing Reynolds number [23]. In this study, the Reynolds number reduces from 0.032 to 0.025 as the porosity increases from 0.41 to 0.7. Therefore, the impact of Reynolds number on $\bar{F}_v / \bar{F}_p$ can be neglected here. The variance of the viscous to pressure component ratio remains almost constant as the porosity reduces. For example, most particles have $\bar{F}_v / \bar{F}_p$ in [0.1, 0.4] and [0.3, 0.6] for the samples with porosity $\varepsilon = 0.41$ and 0.5, respectively. Particle angularity tends to reduce $\bar{F}_v / \bar{F}_p$. An increase in D_{2-8} shifts the distribution to the left and slightly increases the variance at each porosity level. We calculated the mean value of viscous and pressure components of fluid-particle interactions and normalized their values with the sample $D_{2-8} = 0.1$ (Fig. 22). Angularity tends to increase the pressure component more dramatically than the viscous component. This is probably caused by the larger variance of the pressure distribution on a more angular particle surface.

5.5. Drag force

The total fluid-particle interaction consists of a buoyant force and a drag force in un-resolved CFD-DEM simulations. Typically, the total fluid-particle interaction, $\mathbf{F}_{f \rightarrow s}$, and drag force, $\mathbf{F}_d$, are correlated with either pressure gradient ∇p or porosity ε through the following equations [57]:

$$\mathbf{F}_{f \rightarrow s} = \mathbf{F}_d - \nabla p V_p \quad (15)$$

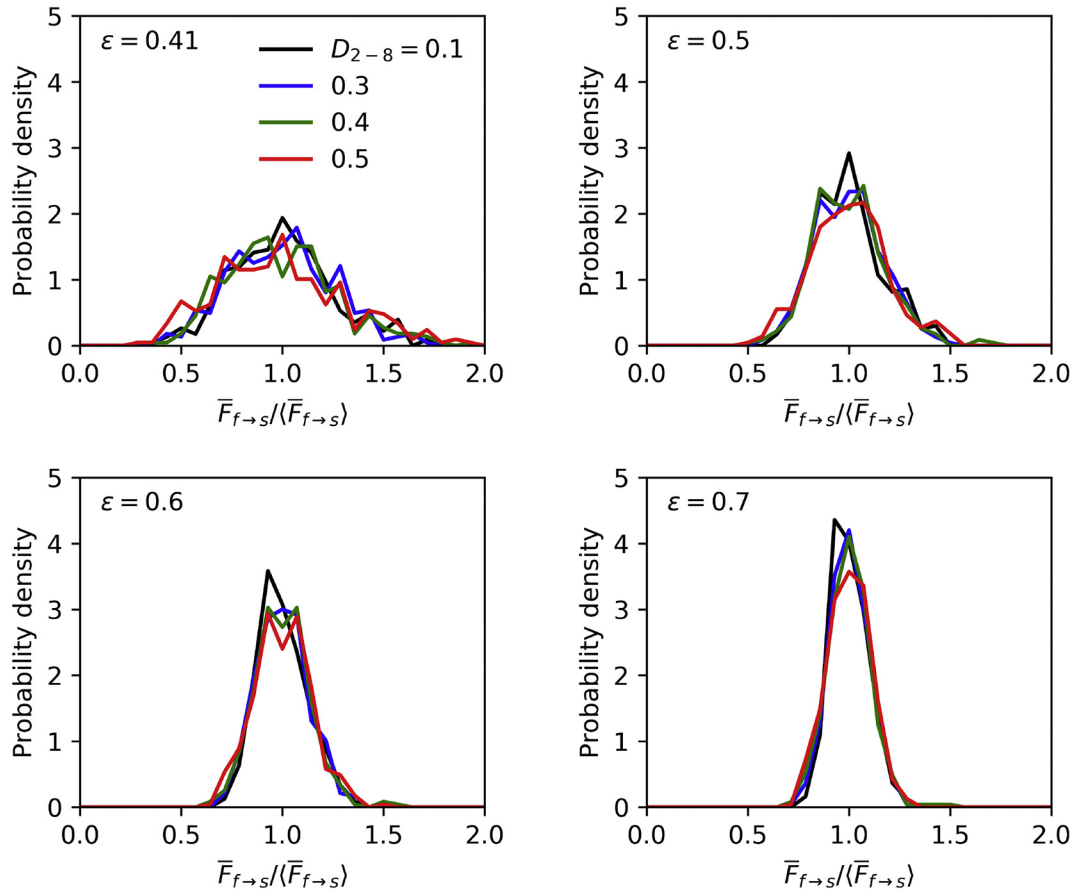


Fig. 19. Influence of porosity and angularity on the distributions of fluid-particle interaction coefficients normalized by their mean values.

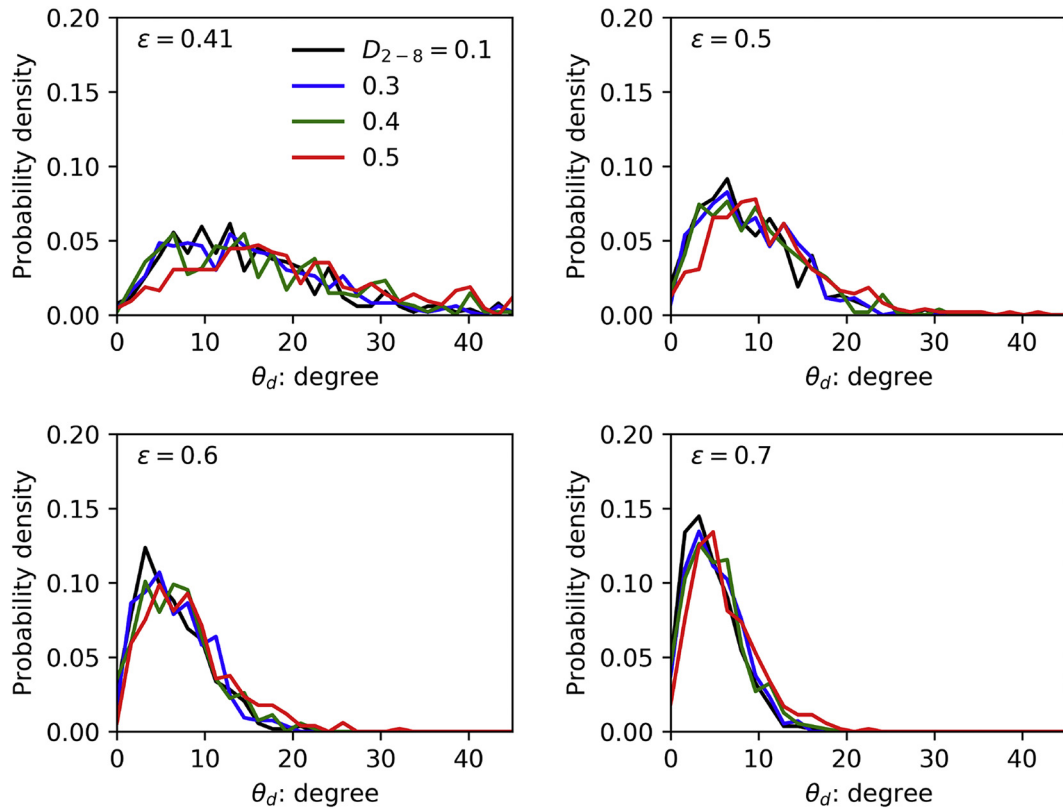


Fig. 20. Influence of porosity and angularity on the distributions of the deviation angle of the fluid-particle interactions from the flow direction.

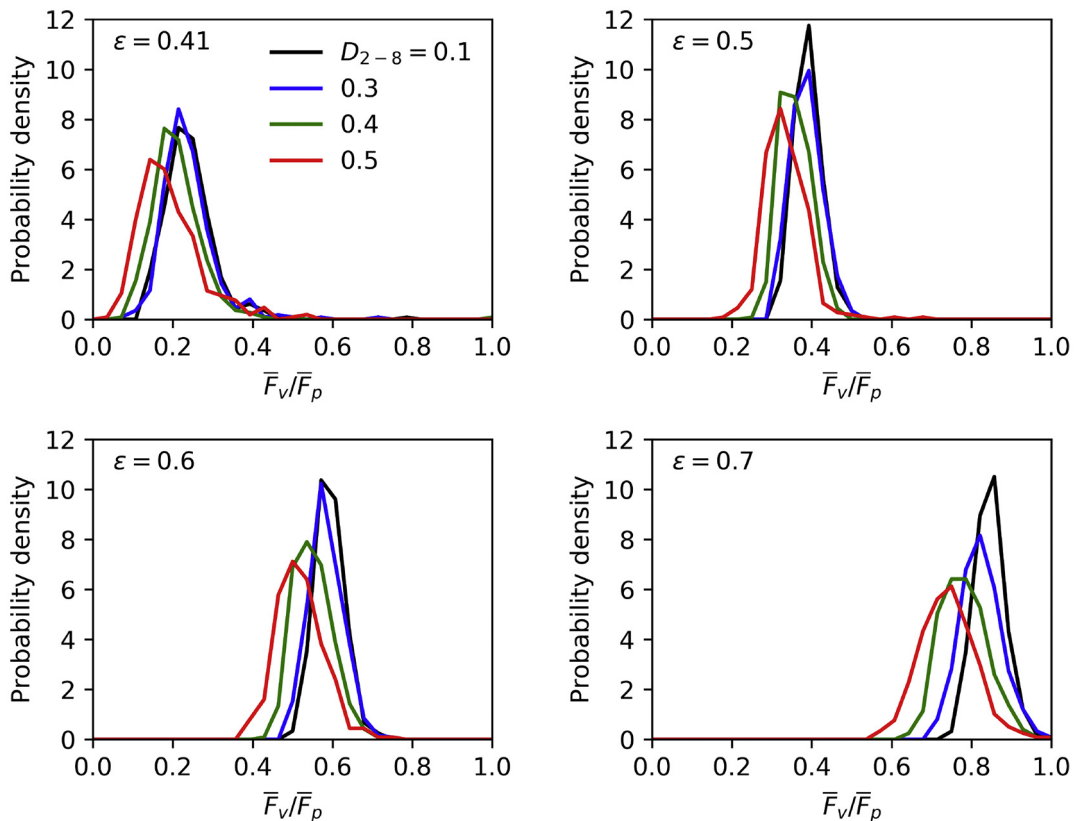


Fig. 21. Influence of porosity and angularity on the distributions of the ratio between viscous and pressure components of fluid-particle interaction coefficients.

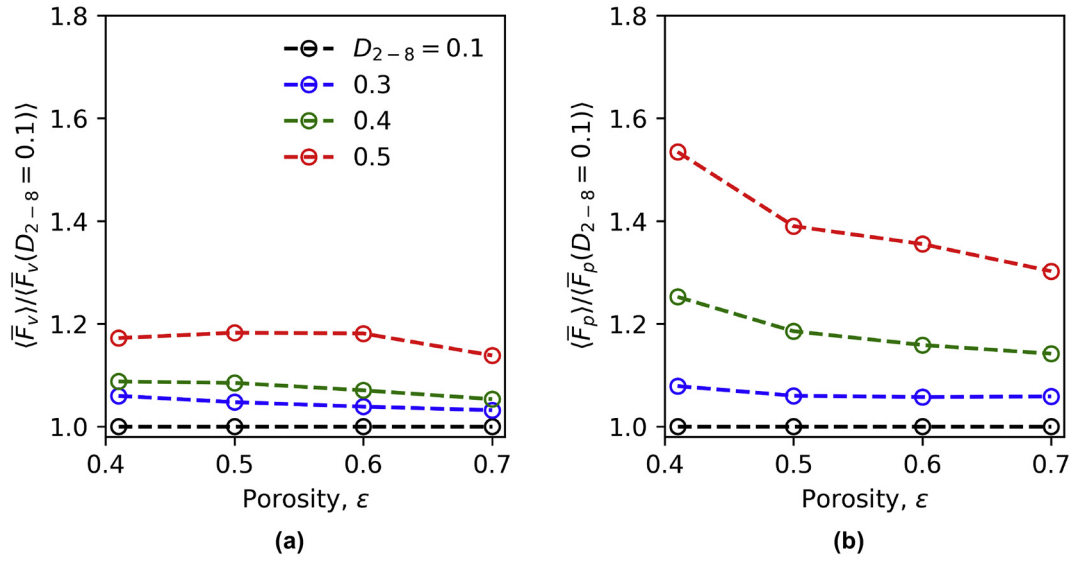


Fig. 22. Influence of porosity and angularity on the mean value of (a) viscous and (b) pressure components of fluid-particle interactions normalized with the sample $D_{2-8} = 0.1$.

$$\mathbf{F}_{f \rightarrow s} = \frac{1}{1-\epsilon} \mathbf{F}_d \quad (16)$$

where p is fluid pressure and V_p is the particle volume. The drag force was estimated from the total fluid-particle interaction through both methods and normalized by Stokes drag force. Fig. 23 shows the influence of porosity and particle angularity on mean drag force. The drag force estimated by both methods is consistent to the equation proposed by Hoef et al. [57] for particles with $D_{2-8} = 0.1$:

$$\bar{F}_{d, Hoef} = \frac{10(1-\epsilon)}{\epsilon^2} + \epsilon^2 (1 + 1.5\sqrt{1-\epsilon}) \quad (17)$$

The drag force increases dramatically as particles become more angular. For the densest packing with $\epsilon = 0.41$, the estimation with Eq. 15 predicted a drag force increase of 69% as D_{2-8} increases from 0.1 to 0.5. The impact of angularity becomes less important as porosity increases, i.e. the increase of drag force is 26% for the loosest packing. This trend is consistent with the total fluid-particle interactions

(Fig. 18b). The variation of drag force estimated by Eqs. 15 and 16 is less than 10%.

5.6. Scaling effect

This study scaled particle size without changing centroidal locations to reach different packing densities. Therefore, we could compare the fluid-particle interaction forces between two particles with the same position in two different porosity levels. As shown in Fig. 24a, the fluid-particle interaction forces normalized by their mean value for two diluted samples tend to form a linear relationship. The rotation from the equivalent line indicates that the particles with $\bar{F}_{f \rightarrow s} / \langle \bar{F}_{f \rightarrow s} \rangle$ higher than one in $\epsilon = 0.7$ sample will have even higher $\bar{F}_{f \rightarrow s} / \langle \bar{F}_{f \rightarrow s} \rangle$ as porosity reduces to 0.6, while the particles with $\bar{F}_{f \rightarrow s} / \langle \bar{F}_{f \rightarrow s} \rangle < 1$ experience the opposite trend. Therefore, the variance of fluid-particle interactions becomes larger as porosity reduces. It demonstrates that the relative positions of particles have a dominant influence on the particle-to-particle variance within one sample, and this influence is porosity-

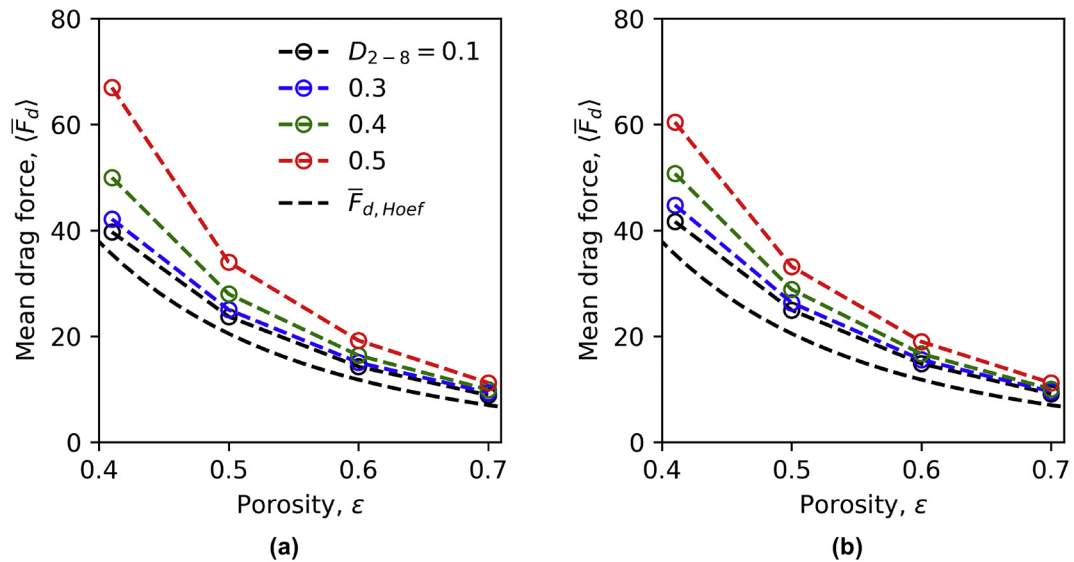


Fig. 23. Influence of porosity and angularity on the mean normalized drag force estimated by (a) Eq. 15 and (b) Eq. 16.

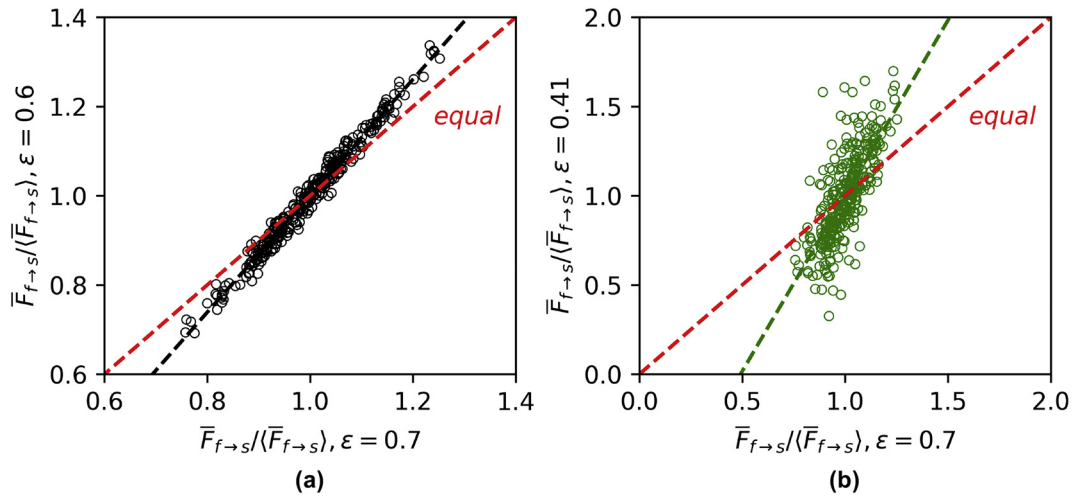


Fig. 24. Influence of particle scaling on the normalized fluid-particle interactions for individual particles (a) between $\varepsilon = 0.7$ and 0.6; (b) between $\varepsilon = 0.7$ and 0.41. The samples have $D_{2-8} = 0.3$.

dependent. A previous study found that the closest four to eight particles, particularly from the particles at the upstream, have the most important influence on a given particle's fluid-particle interaction force [24]. The relationship between the densest packing $\varepsilon = 0.41$ and loosest packing $\varepsilon = 0.7$ has much larger variance (Fig. 24b). For example, the particles with $\bar{F}_{f \rightarrow s} / \langle \bar{F}_{f \rightarrow s} \rangle = 1$ for $\varepsilon = 0.7$ sample could have a $\bar{F}_{f \rightarrow s} / \langle \bar{F}_{f \rightarrow s} \rangle$ between 0.5 and 1.5 in the $\varepsilon = 0.41$ sample. This large variance indicates a more complex flow field in dense packing that affects the particle-to-particle variance of fluid-particle interactions.

6. Conclusions

This study has investigated seepage flow in packings of angular particles. Spherical harmonics were used to randomly generate irregular-shaped particles with different levels of angularity. Dense packings were constructed by gravity deposition of irregular clumps in DEM. The clumps were generated by an efficient overlapping sphere generation code that combines image processing and optimization methods. Loose packings were obtained by scaling down the particle size. We estimated flow fields and fluid-particle interactions through CFD simulations for the packing geometries with various porosity and particle angularity. The fluid-particle interactions obtained from the CFD model were validated with regular packings.

The Kozeny-Carman equation overpredicts the permeability of the dilute samples, while the Zick & Homsy solutions provide a better estimation of permeability for the samples with a large variance of porosity. Particle angularity has a noticeable impact on permeability, which reduces about 30% as the angularity increases from $D_{2-8} = 0.1$ to 0.5. However, particle angularity has a limited influence on the flow fields and the tortuosity.

More angular particles have larger fluid-particle interactions at the same porosity level, which is consistent with the permeability data. The influence of angularity is more significant for the pressure component of fluid-particle interaction force than the viscous component. A more angular surface topology increases the difference of pressure distribution on a particle surface. Therefore, particle angularity has a localized influence on permeability and fluid-particle interactions with limited impacts on the sample-scale flow fields and tortuosity. Also, angular particles tend to experience a much higher drag force than spherical particles.

The fluid-particle interactions have a large particle-to-particle variance in a sample in terms of both magnitude and direction. This variance

is more significant in denser packings. We made a particle-to-particle comparison of fluid-particle interactions for the samples with different porosity and fixed particle centroids. A linear relationship exists between the fluid-particle interactions of the corresponding particles in different porosity levels for dilute samples. As porosity reduces, the particles with a fluid-particle interaction larger than the mean value tend to have an even higher portion of fluid-particle interaction. The linear relationship also demonstrates the importance of the relative particle positions to determining the particle-to-particle variance of the fluid-particle interaction forces. This relationship has a large variance for dense packings with more complex flow fields.

Nomenclature

A_i	area of surface element i
c_l^n	SH coefficient at degree l and order m
C_{K-C}	Kozeny-Carman empirical coefficient
d_e	equivalent particle diameter
d_l	spherical descriptor at degree l
D_{2-8}	normalized spherical descriptor for degree 2 to 8, an indicator for angularity
F_d	drag force
$\bar{F}_d$	drag force normalized by Stokes' drag which acts in the z -direction
$\bar{F}_{d,Hoef}$	drag force estimated from the Hoef equation normalized by Stokes' drag which acts in the z -direction
$F_{f \rightarrow s}$	fluid-particle interaction force
$\bar{F}_{f \rightarrow s}$	fluid-particle interaction coefficient
$F_{f \rightarrow s}^s$	Stokes' drag force (z direction)
F_p	pressure component of fluid-particle interaction force
$\bar{F}_p$	pressure component of fluid-particle interaction coefficient
F_v	viscous component of fluid-particle interaction force
$\bar{F}_v$	viscous component of fluid-particle interaction coefficient
$\bar{F}_{f \rightarrow s, xy}$	fluid-particle interaction coefficient perpendicular to flow direction
$\bar{F}_{f \rightarrow s, z}$	fluid-particle interaction coefficient parallel to flow direction
k_{KC}	permeability estimated from Kozeny-Carman equation
$\mathbf{n}_i$	normal vector for surface element i
N_{sph}	number of overlapping spheres used to fill irregular particle surface
p	fluid pressure
p_i	kinematic normal pressure on surface element i
$\mathbf{R}_{dev,i}$	deviatoric stress tensor for surface element i

R_f	filling ratio defined as the ratio between filled volume and total particle volume
S_0	specific surface area
T	flow tortuosity
$\mathbf{u}$	flow velocity vector
u	magnitude of flow velocity vector
$\bar{u}_x$	x-direction component of flow velocity vector normalized by seepage velocity
$\bar{u}_{xz}$	projection of flow velocity vector on x-z plane normalized by seepage velocity
$\bar{u}_z$	z-direction component of flow velocity vector normalized by seepage velocity
u_z	z-direction component of flow velocity vector
v	superficial flow velocity
V_p	particle volume
$Y_l^m(\theta, \phi)$	SH at degree l and order m
ε	packing porosity
θ	latitudinal coordinate
θ_d	deviation angle of fluid-particle interaction from macroscopic flow direction
ϕ	longitudinal coordinate
ρ	fluid density
μ	fluid dynamic viscosity
$\langle \dots \rangle$	mean value

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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