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How particle shape affects the flow through granular materials

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Flow through the pores of granular materials has many instances in practice. Therefore, it is interesting to realize how some parameters, such as the shape of the particles affect the passing flow. Following the recent mathematical theory proposed by the authors, this paper deals with the issue of how tortuosity and permeability are influenced by the particle shape. Comparison of the results with the experimental data reveals the competency of the theory in predicting the impact of particle geometry.

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I. INTRODUCTION

Diffusion in granular materials is of primary interest to a large number of researchers in various fields ranging from physics [1] to civil [2], chemical [3], petroleum [4], material [5], mechanical [6,7], food [8], bioengineering, as well as nanotechnology [9]. Tortuosity and permeability are two significant macroscopic parameters of a granular medium that affect the passing flow. Despite being more than 70 years since Carman [10] registered a milestone after modifying the permeability equation of Kozeny [11] by implicitly introducing a tortuosity term, a broad consensus has not been reached on how particle shape affects the passing flow since a robust framework for tortuosity and permeability has not yet been established [12,13]. Following the authors' recently developed mathematical theory of fluid flow in granular media [14], here we show how particle shape and arrangement along with the porosity of the granular medium affect the tortuosity and permeability by presenting closed-form functions that can be applied for the whole practical porosity range. This is a major step forward in comparison to other theoretical or empirical papers that are only valid for a certain porosity range. The quantitative comparison of the present results with those of the literature for different particle shapes shows excellent agreement. The outcomes of this paper are expected to remove some ambiguities regarding diffusion in particulate media and, thus, to favor many disciplines dealing with granular materials.

The investigation of the effect of particle shape on macroscopic properties of granular media probably dates back to 1933 when a semiempirical equation was proposed [15] for the hydraulic conductivity of angular-shaped sands. It was, however, rather ambiguous due to the incorporation of not well-defined shape and packing parameters, and it was limited to sands only. Subsequent empirical papers indicated the significant dependency of permeability on particle shape [16], which was supported through the extensive experimental paper of Wyllie and Gregory [17] on randomly packed particles of different shapes. Although so far, correlations have been proposed to account for the effect of particle shape on permeability, they have neither proved to be successful for different particle shapes nor explicitly taken the characteristic shape parameters of the granules into account [18,19].

The recently developed effective medium theory [14], which is a modification of the original theory by Bachmat and Bear [20] and Bear and Bachmat [21,22], has proven successful in describing the hydraulic tortuosity and permeability of a uniform bed of spheres in a completely analytical framework for two selected arrangements of particles [14]. In the following, the original idea is expanded to allow for different particle shapes and arrangements, and thus, general functions are presented for randomly packed homogenous granular materials.

II. VOLUME AVERAGING APPROACH

Based on the paper of Ahmadi *et al.* [14], permeability of a granular medium can be described as

$$K = \frac{3n\Delta_f^2}{C_f}\frac{T_f^*}{2+T_f^*}, \tag{1}$$

where K and n are permeability and porosity, respectively, and C_f is a constant related to pore size. Also,

$$T_f^* = \frac{\theta^S}{n} = \frac{S_{ff}}{nS_0}, \tag{2}$$

$$\Delta_f = \frac{U_{0f}}{S_{fs}}, \tag{3}$$

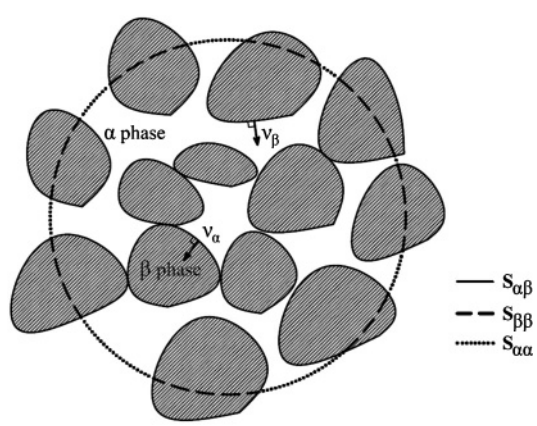

FIG. 1. REV defined in Ref. [14]; α and β denote fluid and solid phases, respectively; $S_0 = S_{ss} + S_{ff}$.

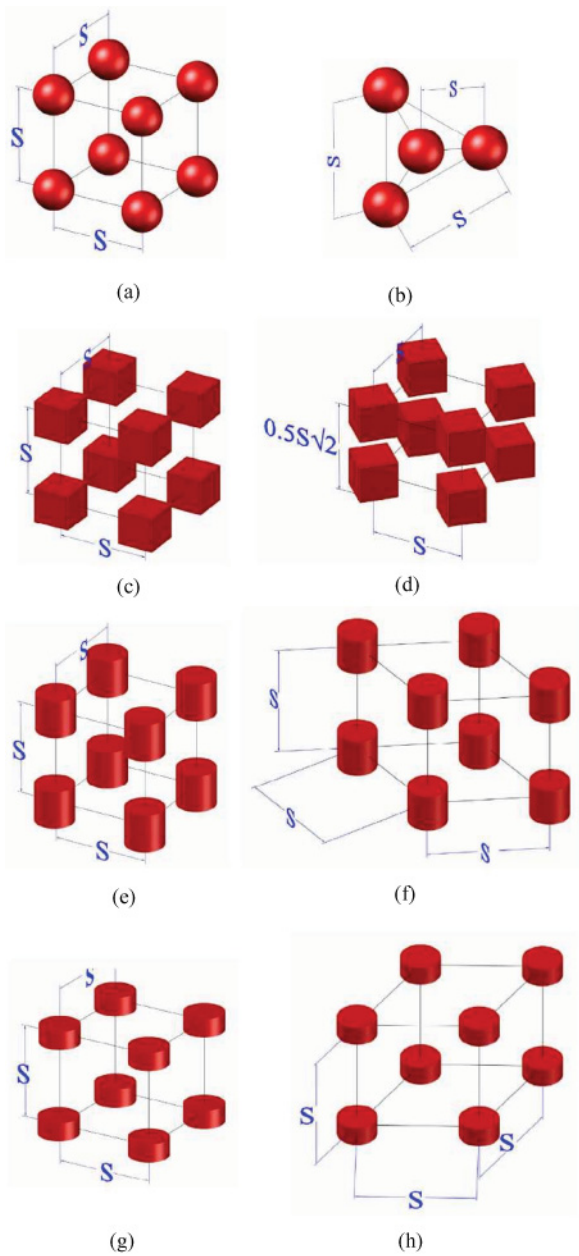

FIG. 2. (Color online) Four sets of REVs for different particle shapes, each set corresponds to two different minimum attainable porosities; (a) and (b) sphere, (c) and (d) cube, (e) and (f) cylinder with length to diameter ratio = 1, (g) and (h) disk with length to diameter ratio = 0.5. For a description, see Table I.

where S_{fs} is the interface area of the fluid and solid phases, S_0 is the total area of the surface around the representative elementary volume (REV), and S_{ff} is the fraction of S_0 along which the fluid is in contact with itself (Fig. 1). The volume of the fluid in the REV is denoted by U_{0f} in Eq. (3).

The methodology explained in Ahmadi *et al.* for the derivation of the above parameters for the cubic and tetrahedral arrays of spheres [14] then is employed herein for the case of an arbitrary REV of identical particles of irregular shape; therefore, after substituting Eqs. (2) and (3) in Eq. (1)

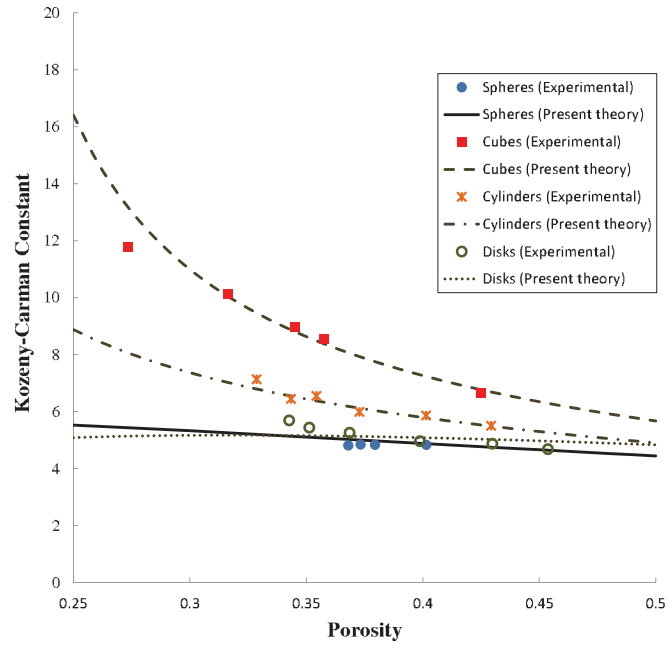

FIG. 3. (Color online) Comparison of the proposed KC function in Eq. (8) and the experimental results of Refs. [16,17].

and comparing it with the traditional Kozeny-Carman (KC) equation, T_f^* is calculated for an arbitrary REV as

$$T_f^* = \frac{1 - B_{\text{array}} B_{\text{compactness}} (1-n)^{2/3}}{n}, \tag{4}$$

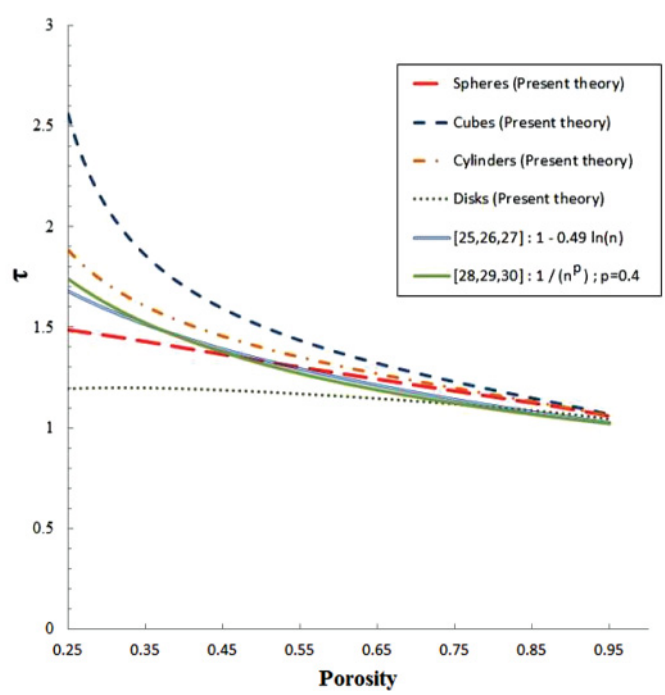

FIG. 4. (Color online) Comparison of the tortuosity results from the proposed function in Eq. (7) for different particle shapes with two well-established empirical correlations for spherical particles (see Refs. [25–30] for information regarding the data represented by the solid lines).

TABLE I. Summary of $B_{\text{compactness}}$ values for packings of particles of different geometric shapes and arrangements.

Particle shape	Array	Minimum attainable porosity	$B_{\text{compactness}}$
Sphere	Cubic (a)	0.476	0.250
	Tetrahedral (b)	0.260	0.229
Cube	Cubic (c)	0	0.167
	Rhombohedral prism (d)	0.5	0.210
Cylinder	Cubic (e)	0.215	0.197
	Rhombohedral prism (f)	0.093	0.187
Disk	Cubic (g)	0.215	0.179
	Rhombohedral prism (h)	0.093	0.174

where the compactness term, $B_{\text{compactness}}$, is one of the two three-dimensional shape descriptors introduced by Lin and Miller [23] based on x-ray microtomography papers for characterizing irregular particles,

$$B_{\text{compactness}} = \frac{S_p}{V_p^{2/3}}, \tag{5}$$

in which S_p and V_p are the surface area and the volume of a particle, respectively.

The other parameter in Eq. (4), namely, $B_{\text{compactness}}$, depends on the arrangement of particles as well as their aspect ratio (as the second shape descriptor in Ref. [23]), which is discussed subsequently.

Replacing Eqs. (3) and (4) in Eq. (1) yields the following permeability equation for an arbitrary REV:

$$K = \frac{3}{C_f}\frac{1 - B_{\text{compactness}}B_{\text{shape}}(1-n)^{2/3}}{2n + 1 - B_{\text{compactness}}B_{\text{shape}}(1-n)^{2/3}} \times \frac{n^3}{(1-n)^2}\frac{1}{S_s^2}, \tag{6}$$

where S_s is the specific surface of a particle.

By analogy with the traditional KC equation of $K = \frac{n^3}{\kappa S_s^2(1-n)^2}$ where $\kappa = C_f\tau^2$ is the so-called KC constant, the tortuosity function is written as

$$\tau = \sqrt{\frac{2n}{3[1 - B_{\text{compactness}}B_{\text{shape}}(1-n)^{2/3}]} + \frac{1}{3}}, \tag{7}$$

and

$$\kappa = C_f\left(\frac{2n}{3\left[1 - B_{\text{compactness}}B_{\text{shape}}(1-n)^{2/3}\right]} + \frac{1}{3}\right). \tag{8}$$

In addition to many experimental observations, it is clear from the above equation that the KC parameter is not a constant and consists of two terms: the second term $(C_f/3)$ is a constant, whereas, the first one depends on the porosity and the two introduced B parameters.

The parameter $B_{\text{compactness}}$ for the tetrahedral and cubic packings of spherical particles, as derived analytically [14], is 0.229 and 0.250, respectively, which correspond to invariant geometric arrangements of the particles, i.e., tetrahedral and cubic packings remain tetrahedral and cubic when the porosity changes. The porosity change within each configuration is maintained through the variation in S in Fig. 2. This also holds true for other particle shapes in the figure. Table I shows the minimum attainable porosities corresponding to four sets of particle arrays, each set containing two arrays with a particle shape.

III. VERIFICATION

Dependency of packing characteristics on porosity and particle shape has been studied by many researchers, e.g., in Zou and Yu [24], and has been explained mostly in terms of the triple relation among sphericity, porosity, and particle shape. Taking $B_{\text{compactness}}$ as an alternative to sphericity and assuming a linear relation between $B_{\text{compactness}}$ and porosity for each set of particle shapes in Table I, different analytical relations are obtained, as defined in Table II. These relations then are modified to better match the proposed KC function [Eq. (8)] with the experimental results of Refs. [17,18] as depicted in Fig. 3. Good agreement is found for all particle shapes. Comparison of the $B_{\text{compactness}}$ relations before and

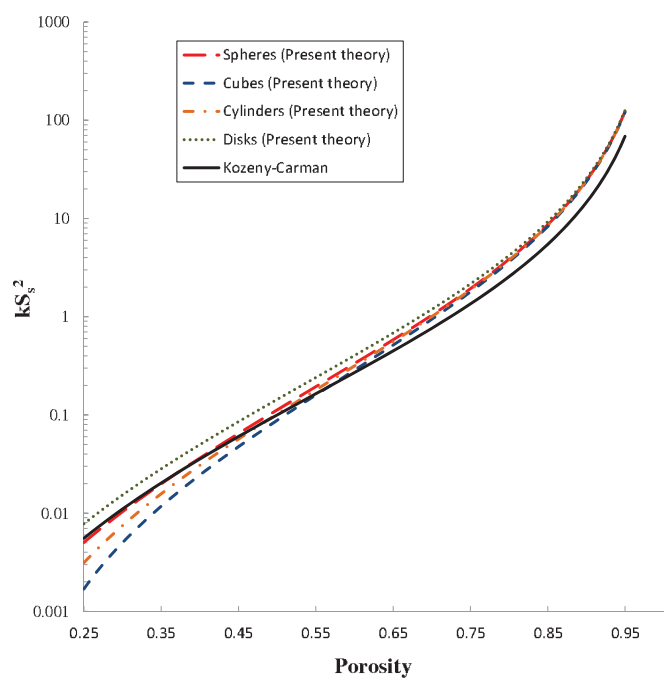

FIG. 5. (Color online) Comparison of the permeability results from the proposed function in Eq. (6) for different particle shapes with the Kozeny-Carman equation.

TABLE II. Analytical relations for $B_{\text{compactness}}$ for different particle shapes and their experimentally based modifications.

Particle shape	Analytical relation for $B_{\text{compactness}}$	Modified analytical relation for $B_{\text{compactness}}$ based on the experiment
Sphere	$0.097n + 0.204$	$0.097n + 0.204$
Cube	$0.086n + 0.167$	$0.090n + 0.174$
Cylinder	$0.082n + 0.179$	$0.082n + 0.187$
Disk	$0.041n + 0.170$	$0.041n + 0.165$

after modification in Table II revealed only slight modifications for cubic-, cylindrical-, and disk-shaped particles, whereas, spherical particles needed no change. The reason for this can be attributed to the distinction between spheres and other particle shapes in view of shape descriptors. While sphericity or compactness is the only necessary descriptive feature for a sphere, the aspect ratio, as the second shape descriptor in Ref. [23], becomes important for shapes other than the sphere.

Tortuosity values for different particle shapes are compared with each other and the two accredited tortuosity correlations for spherical particles in Fig. 4. Again, the results cohere well.

From Fig. 4, an important finding is the convergence of the tortuosity diagrams for different particle shapes when porosity increases. While the difference between the highest and the lowest tortuosities in the figure (pertaining to cubes and disks, respectively) is more than twofold at $n = 0.25$, it drops dramatically when the porosity exceeds 0.5 and nulls near the upper porosity limit of 1. This clearly illustrates the dominance of particle shape in low and midporosity ranges.

The effects of different particle shapes on permeability, nevertheless, are less tangible for most porosity ranges as depicted in Fig. 5. They become significant only at low porosities with the disks and cubes having the highest and lowest permeabilities, respectively, among the others.

IV. CONCLUSION

Here, analytical functions have been presented based on the recent volume averaging theory proposed by the authors to allow for the effects of particle shape on tortuosity, porosity, and the Kozeny-Carman constant. Although regular arrays are contemplated in this paper, in contrast to unstructured arrangements in physical experiments, the results are consistent with the well-established empirical data and correlations in the literature. The findings of the present paper can be utilized in various fields dealing with granular materials.

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