



Particle Morphology Effect on the Soil Pore Structure

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Abstract. The soil fabric can be expressed as a network model. Granular media voids connectivity and constriction size distribution may lead to movement of air, fluids, and solids in the soil, and therefore affect the chemical, physical and mechanical properties of soils. Understanding the soil voids areas and their inter-connection might be helpful in understanding different phenomena such as transport in porous media, water retention, fluid flow in the soil, soil contamination, internal erosion, suffusion, and filtration. In addition, specifying the soil voids interconnectivity can help researchers and practical engineers to provide the best rehabilitation and remediation approaches. The pore network was investigated in the current study, assuming the soil particles to be similar to discrete spheres and particles with different shapes. Also, based on the modelling techniques, the profiles of pore connectivity and constriction size distribution were assessed.

Keywords: Soil structure · Soil fabric · Pore network model · Constriction size distribution · Particle shape

1 Introduction

The porous medium can be considered as the interconnected networks of bonds and nodes. The nodes represent the pores, and bonds show constriction between these pores. Fatt [1] pioneered to use of two-dimensional square and regular networks, including cross-sectional pipes with various radii, to describe the stone pore structure [1]. The physics of air and fluid flow and soil mass transport can be simulated using the network model [2]. Network modelling is one of the methods that can be recruited to estimate the transport in porous media [1–5], fluid flow in porous media and permeability [6, 7] and the amount and size of eroded particles from soil skeleton [7–11]. A pore network should specify the geometric characteristics and topology of porous media. In order to conduct an accurate simulation of the porous media, the nature of the convergence and divergence of pore distribution, multiple connectedness of pore space, and pore size distribution should be considered [12]. In practice, a network model can be created by average connectedness (coordination number), pore size distribution, and pore length

distribution [3]. The regular networks, such as those comprised of square shapes or honeycomb forms, cannot describe irregular soils and rock structures due to those real amorphous and tortuous structures. By changing the length or removing some of the constrictions, a network similar to the actual soil structure voids can be created. Voronoi and Kylie lattice are two examples of these networks. Based on the network configuration and the coordination number, different networks can be generated. Figure 1 illustrates some examples of two-dimensional networks of soil and rock pore structures, bonds, and nodes which are equivalent to the soil pores and the paths of their connectedness in these networks, respectively. The coordination number (Cn) can describe this relationship, which represents the bonds connected to each node [2].

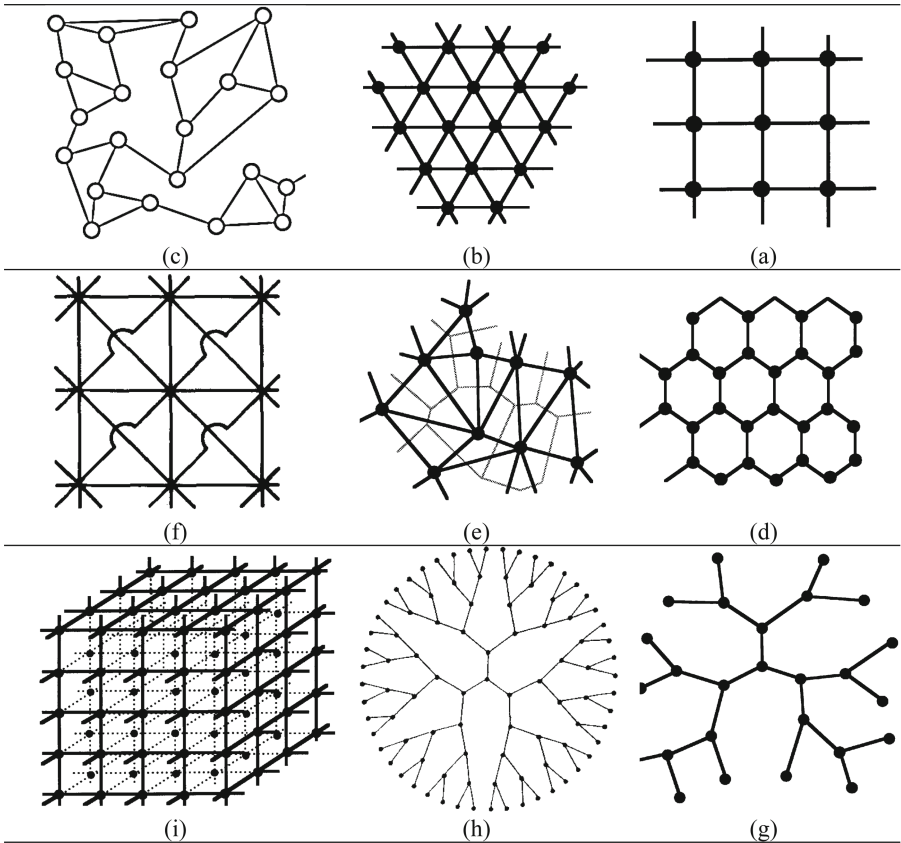


Fig. 1. Examples of the bi-dimensional networks, (a) square network, Cn = 4, (b) rectangle network, Cn = 6, (c) irregular network, Cn = 3, (d) hexahedral network, Cn = 3, (e) Voronoi lattice, Cn = 4, (f) intercept square network, Cn = 8, (g) Kylie lattice (simple graph), Cn = 3, (h) Bethe lattice, Cn = 3, (g) cubic network, Cn = 6. [3, 13–16]

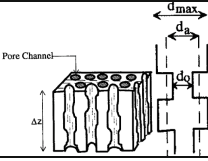
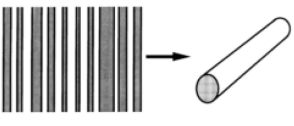
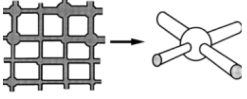
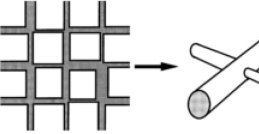
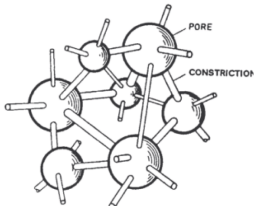
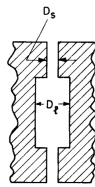
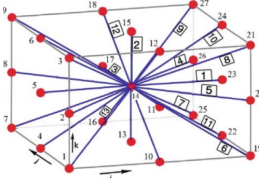
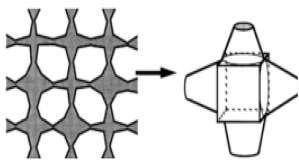
The shape of the pores can be spherical, cylindrical, incomplete conical, crossed, bubble-shaped, similar to concrete pores, or flat such as mica or clay. However, pores

mostly have irregular shapes [17]. Pore geometry and its tortuosity and topology play a significant role in the structure of porous media [18]. The coordination number can be considered as the main feature of network topology. A network model should determine the mean of the coordination number, the topology of pore connectivity on the microscopic scale, and its distribution [14, 19]. The coordination number of the different proposed networks ranges from 1 to 26. Raouf and Hassanizadeh [19] proposed a three-dimensional cube network, in which each pore has 13 outputs in different directions, and its coordination number is 26. The network models can be divided into quasi-static and dynamic displacement types [20]. Quasi-static models create a capillary pressure in the network and calculate the final static position of fluid-liquid interfaces. An inflow rate is usually applied in dynamic models, which relates the transient pressure and interface position.

In order to describe each network element, some parameters such as radius, shape factor, volume, area, and length should be determined [21, 22]. It is difficult to measure and calculate these parameters due to the complexity and amorphous of the porous medium; however, these parameters are calculated for mono-spheres [23, 24]. Regular and irregular models of the proposed pore network for simulating soil structure are shown in Table 1. Some of these models were suggested to mimic fluid flow in porous media; the model of the proposed network tube of Fatt [1], the ball and tube network model of Chandler et al. [25], Raouf and Hassanizadeh [19], Indraratna & Vafai [8], Kovacs [7], conical pore and tube Network Model of Toledo et al. [2].

Primary constrictions for fluid flow are through the pore throats, where pores interconnect with each other. In sediments, the dimension of the two interconnected pores might specify the constriction size or the pore throat size (d_{throat}) is typically half of the pore dimension (d_{pore}). The following geometric relations apply to a simple cubic packing of monosized spheres: $d_{pore} = 0.73d_{grain}$, $d_{throat} = 0.41d_{grain}$ and $d_{throat} = 0.56d_{pore}$. So the correlation between k -and- d_{pore} can be extended to k -and- d_{throat} , applying an appropriate correction factor [30]. In the diagenetically altered, and sedimentary structures, the pore and constriction size ratio may deviate apparently from $d_{throat} \approx 0.5d_{pore}$ [31]; thus, considerations must be taken into account for the constriction size. For example, the hydraulic conductivity of carbonates can be associated with the square of the maximum constriction size ($\max[d_{throat}]^2$) and maintain the quadratic relation in Hagen-Poiseuille [30]. The soil porosity relies on different parameters, including packing density, the extent of the particle size distribution (polydisperse cases versus monodisperse ones), the particles shape, and cementation conditions. Three-dimensional pore space networks of the particles were obtained through direct imaging, usually through computed tomography, micro-CT, use of a probabilistic method to produce a synthetic three-dimensional structure that obtains its properties from two-dimensional thin sections, and the simulation of particle packing by using geological processes such as sedimentation and compaction [32]. In the next section, a review of the previous studies including sedimentation method, analytical method, numerical method and experimental methods are presented. Additionally, CT scan image and replica technique are implemented in the current research on the pore soil structure characterization.

Table 1. Pore structure network model

Schematic of pore network	Pore network model	Reference	Schematic of pore network	Pore network model	Reference
	tri-dimensional - parallel tubes	[7, 8]		One-dimensional - parallel tubes	-
	bi-dimensional - ball and tube	[25]		tri-dimensional - tubular	[1]
	tri-dimensional - ball and tube	[29]		One-dimensional - parallel tubes	[27, 28]
	tri-dimensional - ball and tube	[19]		bi-dimensional - conical pore and tube	[30]

2 Methodologies

2.1 Sedimentation Method

Sherard et al. [33] estimated the diameter of the flow channels by collecting the suspended particles in the water passing through the samples. Kenney *et al.* [9] also determined the diameter of the particles passing through the filter by the dry-vibration method. This method is effective for sand filters. Soria et al. [34] evaluated the performance of a filter with the same materials and variable thickness. In this method, base materials were suspended in the filter with a constant head, and passed particles were collected and graded [10, 11]. The diameter of the passing particles might indicate the distance of the particles moving within the filter, based on which Soria et al. [34] recommended a method for specifying the constriction size distribution (CSD).

2.2 Analytical Method

In the analytical method, CSD can be calculated by using PSD. A more realistic structure of the pores can be estimated by considering the relative density and using a probabilistic pattern for particles arrangement [35]. In this case, soil particles are often assumed as spheres. Spherical particles can be considered due to the simplicity and applicability of the calculations and modelling of a large number of particles. Silveira [36] provided a model of spherical particle placement in the densest and loosest state and estimated the size of the eroded particles from the filter. Soil porosity depends on several factors, including density, particle size distribution, shape, and cementation [37]. By simulating the soil with equal size spherical and geometric calculations, soil porosity, n , range between 0.26 and 0.48 based on the arrangement of the particles.

2.3 Numerical Method

Uniform spheres packing has been commonly studied in conditions of random loose and dense packing. However, due to a significant increase in the computation power recently, modelling of more complicated and, simultaneously, realistic particles have become widespread. Thus, large packs of irregular particles can be modelled and analyzed. Utilizing the discrete element method (DEM), the samples with different porosity can be constructed, and the pore network and soil structure are examined [38]. However, creating samples with various shapes in the DEM method is rather difficult. Using the clustering and clumped forms, it would be possible to create various complicated particle shapes by putting spherical particles into a group.

2.4 Experimental and Imaging Techniques

Mercury porosimetry is one of the most common methods for measuring the pore structure of porous materials. This method only characterizes the pore size distribution connected to the mercury reservoir and does not measure the closed pore. This method is usually used to measure pore sizes of 3 nm to 100 μm [3]. The gas absorption method is another approach, which works based on surface absorption and pore surface measurements. This method measures lesser pore size ranges compared with mercury porosimetry [39]. Larger pores of porous media can be measured using 3D imaging or replica technique, by which the results are transferable to finer soils because of the similarity of structure and shape of grains [40]. The samples' three-dimensional imaging can be implemented using a 3D laser scan or micro CT scan (μCT). μCT is a non-destructive method that can determine pore space topology and the skeleton using computed tomography [5]. In addition, nuclear magnetic resonance can be used to quantify the pore structure [41]. Also, three-dimensional images of pores can be created by using statistical reconstruction of two-dimensional images of the thin section of the sample. Several 2D view images of cross-sections from a 3D image can also be produced (as shown in Fig. 2). These images show pore space topology, pore-connectivity, and porosity of samples.

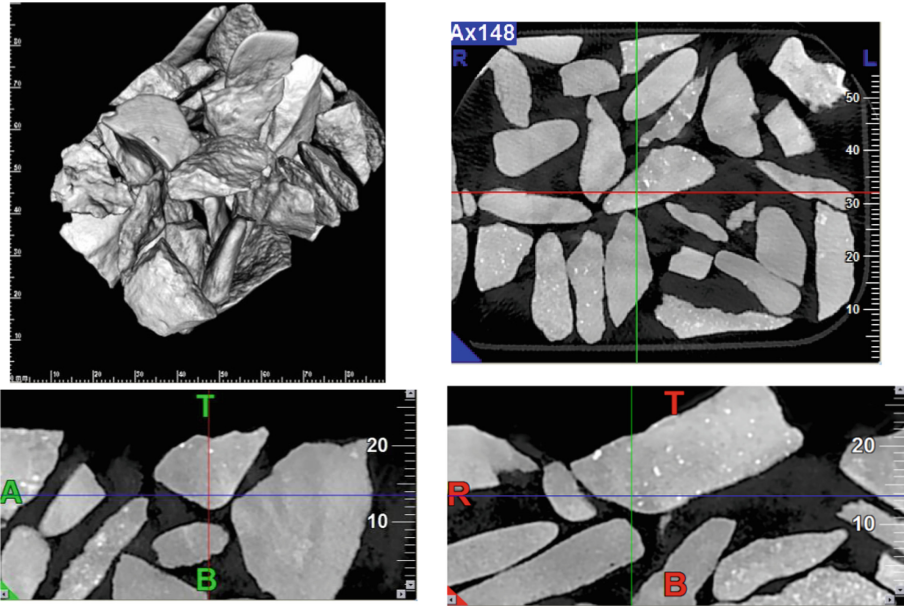


Fig. 2. CT scanning 3D image and cross-sectional 2D images, (R: right, L: left, T: top, B: bottom)

3 Experiments Using Replica Technique

In order to make a model of the coarse-grained pore structure, the liquid resin with high elastic properties enters into the pore until it is saturated. When the resin is hardened, the particles can be removed from the elastic structure, and thus a trace remains from the pore structure. It can also be submerged with resin, slurry, or ceramic powder, deposited in the fluid or immersed in the paste [40]. Sherard et al. [33] filled gravel pores with molten wax and cut the sample after the wax was hardened to examine the channel pores of the gravel.

Following the mentioned pore network modelling using replica technique, an imprint of the pore space for four uniformly graded gravel includes Spherical, Angular, Subangular, and flaky particles, replicated as shown in Fig. 3. Patterns or imprints of the pore network and individual pores show pore geometry, pore number per volume, pore size distribution, and constrictions number per pore (coordination number).

4 Result and Discussion

The acquired results indicated that the particles sphericity or roundness reduction might lead to mean pore length decrease, the tortuosity increase, and constriction sizes reduction [10]. In the case of dealing with flaky and elongated particle samples, the particle arrangement had a higher contribution to pore size distribution than that of specimens with rounded or crushed grains. In these samples, grains' flatness and orientation affected the pores network, whether the grains are placed on their largest, medium, and smallest face or oriented.

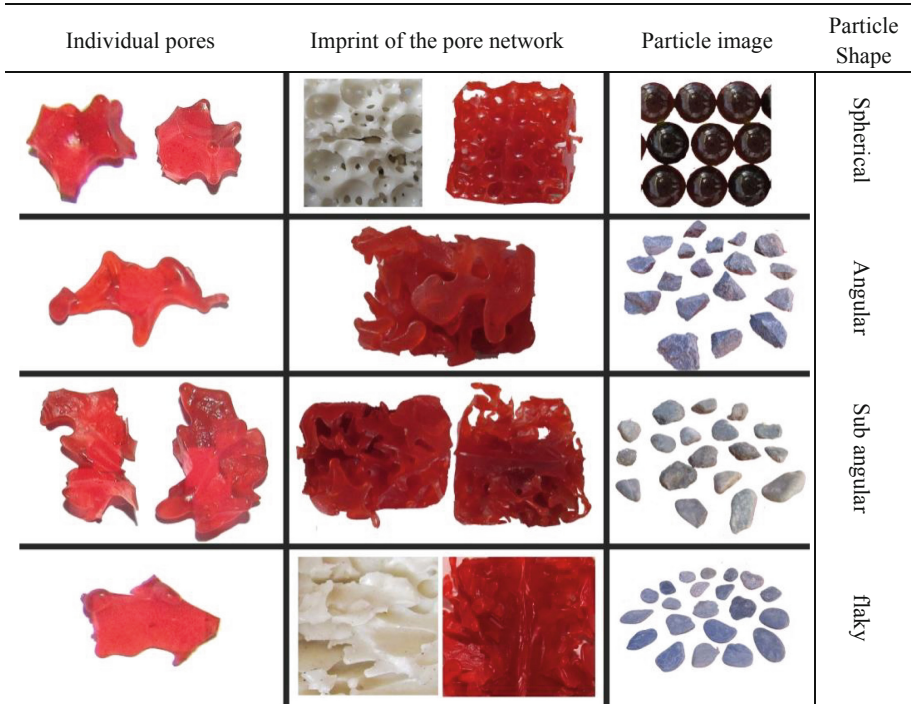


Fig. 3. Pore space imprint for various particle shape

The average coordination number, pores connection and constriction size distribution, pore length, and the tortuosity coefficient should be determined for soil structure description. These parameters are measured using three methods: computed tomography, modeling by discrete element method, and laboratory tests. The shape of most soil particles can be simulated with spherical, pyramidal, cubical, and flaky particles. The soil structure was evaluated by assuming that particles were spherical, rounded, angular (cubical, pyramidal), and flaky [42]. Analytical methods examined the soil structure for spherical particles of different sizes and densities. Nevertheless, the structure of soils with hetero-shaped particles is complex. Determining pore size distribution becomes impossible by increasing the coefficient of uniformity of the soil (C_u) and density changes. However, by probabilistic methods, an equivalent soil structure can be estimated.

For monospherical particles, the coordination number is between 6 and 12, and the centres of the layers vary between 1.41 and 2.0 times the radius of the particles. The length of the path is a function of the diameter of the particles. In addition, porosity is 25.55 and 47.64 for the densest and loose conditions, respectively. Regarding spherical particles with two-size, three-size, and four-size, both the sample density and the arrangement of particles are essential. The pore network of these materials is similar to spherical particles, although the probability of the placement of the particles near each other makes it impossible to calculate the soil structure accurately. As the angularity of the particles increases, the irregularity of the soil structure and the tortuosity path increase. In

addition, the probability of such phenomena as particle bridging and particle breakage in high-pressure increases. Specific surface area (SSA) and shape coefficients differences in flaky specimens can be associated with variations in particle thickness, where thickness increase leads grains SSA to be reduced.

On the other hand, gravity plays another role in packing flaky particles than elongated particles, mainly due to the centre of mass finding lower energy states more easily [43]. The arrangement of the particles in these types of soils plays the most significant role in the pore structure. The placement of the particles on the largest, medium, smaller side or its inclined placement greatly influences the pore network.

5 Conclusion

An imprint of pore space of four uniformly graded gravel includes spherical, angular, subangular, and flaky particle produced, and pore geometry has been evaluated. The analytical method usually can be used for spherical particles, for natural soils, analytical methods should consider and qualify the angularity elongation and roughness of grains.

In the current study pore structure of granular soils and methods to visualize, analyze, simulate and describe the structure of porous media by assuming the soil particle similar to the discrete sphere and particles with different shapes have been presented and discussed. Further, pore network and constriction size distribution were studied using experimental replica technique, and CT-Scan imaging.

An imprint of pore space of four uniformly graded gravel includes spherical, angular, subangular, and flaky particle produced, and pore geometry has been evaluated. Imprints of the pore network and individual pores show pore geometry, pore number per volume, pore size distribution, and constrictions number per pore (coordination number). As the sphericity of the particles decrease, the irregularity of the soil pore structure and the tortuosity path increase.

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