Pore Scale Study of the Influence of Particle Geometry on Soil Permeability

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Abstract

The permeability of a saturated porous medium is an important parameter in the field of water resources and geotechnical engineering. The geometric characteristics of a porous medium are key factors in the prediction of its permeability. In this paper, particles of different shapes are constructed by Cellular Automata (CA) random growth model, and particles with different surface characteristics are constructed by the spherical harmonic function. Then, porous media of different porosities, shapes, surface features, and particle size distributions are generated on the basis of the constructed particles. Three-dimensional Lattice Boltzmann Method is used for the pore-scale simulation of the seepage flow in a porous medium. The numerical results show that the effects of the particle shape and surface characteristics on the permeability are too obvious to be ignored. Using strict univariate analysis, the sensitivity of the various factors to the permeability, ordered from large to small, is as follows: porosity>particle size distribution>particle surface>particle shape. Based on numerical studies, a modified Kozeny–Carman (KC) formula is proposed by considering all the geometrical factors. All the parameters (the Wadell sphericity S_w , Cox roundness R_c , coefficient of non-uniformity C_u , the curve coefficient of curvature C_c , and effective particle size d_{10}) in it are easily obtained in engineering practice and the accuracy of the formula is verified. Although It has been proven that the KC formula is applicable to multi-dispersed spherical particles and non-spherical particles whose surfaces are not very rough, its applicability to rough particles is limited. The modified KC formula does not have this limitation; therefore, it has a wider scope of application than the conventional KC formula.

Keywords: Lattice Boltzmann method; permeability coefficient; particle geometry; CA random growth model; spherical harmonic function.

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9 1. Introduction

10 Several scientific and engineering fields such as water resources, petroleum science, geotech-
 11 nical engineering, and environmental engineering require reliable prediction of the permeability
 12 of saturated porous media (Harr, 2012). Because permeability mainly depends on the geometric
 13 characteristics of a porous medium, geometric parameters can be used to predict the permeabil-
 14 ity when an exact relationship between them is established.

15 After Seelheim (1880) reported that permeability should be related to the squared value of
 16 the characteristic pore diameter, numerous formulas were proposed in the subsequent centuries
 17 to predict the saturated permeability based on geometric parameters. For example, the Terza-
 18 ghi formula (Terzaghi et al., 1996), Hazen formula (Hazen, 1911), Kozeny formula (Kozeny,
 19 1953), Kozeny–Carman formula (KC formula) (Carman, 1937, 1956), and some empirical for-
 20 mulas (Harleman et al., 1963; Beyer, 1964; Vukovic and Soro, 1992; Jabro, 1992; Alyamani and
 21 Sen, 1993; Barr, 2001; Chapuis and Aubertin, 2003; Chapuis et al., 2005; Zhu, 2010; Su et al.,
 22 2014) were proposed based on experimental data. Analyses of the abovementioned empirical
 23 formulas have shown that different methods of calculating the permeability result in significant
 24 differences between the formulas. The simplest of them, the Hazen formula, and the formula
 25 proposed by Harleman et al. (1963) considered only the influence of the effective particle size
 26 d_{10} . The effective particle size and porosity are considered in the Terzaghi formula, Kozeny for-
 27 mula, and the empirical formulas proposed by Vukovic and Soro (1992); Chapuis et al. (2005).
 28 Some empirical formulas have established the correlation between permeability and d_{10} , d_{50}
 29 (Alyamani and Sen, 1993), whereas some do not contain geometric and physical parameters
 30 such as particle size and porosity but establish the relationship between permeability and the
 31 percentage content of sand, silt, and clay (Jabro, 1992; Onur and Shakoor, 2015). Some empir-
 32 ical formulas consider the effects of the gradation parameters C_u and C_c while considering the
 33 particle size and porosity (Beyer, 1964; Zhu, 2010; Su et al., 2014). All the above formulas do
 34 not consider the morphological characteristics of the particles. The KC formula and some em-
 35 pirical formulas are established by introducing the solid specific surface area with consideration
 36 of the porosity (Barr, 2001).

The existing experimental studies show that the KC formula is the most accurate in predicting the permeability (Chapuis and Aubertin, 2003). The classical form of the KC formula is

$$K = C_{KC} \frac{\phi^3}{(1 - \phi)^2} \frac{1}{S^2}, \quad (1)$$

where C_{KC} is an empirical constant, ϕ is the porosity, and S is the specific surface area. The classical KC formula is used to predict the permeability based on two parameters—porosity and specific surface area. The specific surface area is not a basic geometric parameter that varies with the shape, surface characteristic, and gradation of the particles. Some approaches are available in literature to measure the specific surface area. Several Digital Image Processing (DIP) algorithms can calculate the specific surface area of a porous medium using its micro images obtained by Computed Tomography (CT) (Lindquist et al., 1996; Song et al., 2001; Porter et al., 2010). Some experimental methods such as the gas adsorption-based method can also be used to estimate the specific surface area (Scheidegger, 1958; Collins, 1976). However, both DIP based and experimental methods can only be applied to some specific samples. It is not as easy to perform statistical averaging of the specific surface area as that of the basic geometric parameters of particles, such as sphericity, roundness, and gradation. In many cases, it is more difficult to measure the specific surface area than the basic geometric parameters, which limits the application of the KC formula. Moreover, the constant C_{KC} in the KC formula is not actually a constant without considering the tortuosity (Kaviany, 2012), and the accuracy of the KC formula for a porous medium with low porosity or rough particles is questionable.

In summary, although there are many formulas for predicting the permeability using the geometric parameters, only a few of them can be used in engineering practice. The Hazen formula and the Terzaghi formula are simple, but their accuracy is not sufficient for engineering practice (Carrier, 2003). The empirical formulae proposed in the existing studies are diverse without a general format, as these can be applied only to special soils (Rosas et al., 2014). Although the KC formula has higher accuracy, its application is limited because the specific surface area is an indirect geometric parameter.

The investigation of the effect of basic geometric characteristics of particles on the permeability and the establishment of an accurate prediction formula using easily available parameters are critical research issues. The limitation of an experimental study is that the change in a single variable cannot be strictly controlled in an experiment, especially to ensure that the porosity of the soil sample does not change. The porosity of soil usually changes when the particle size and gradation change. Therefore, different researchers conducting experiments with different materials have reported different results, and some have even reported contradictory conclusions (Su et al., 2014; Kong et al., 2011). Another limitation of the experimental study is that the seepage process is not visible and the mechanism of permeability cannot be studied on the pore scale.

Numerical simulation can overcome the shortcomings of material disunity and improper variable control in experiments. However, the traditional numerical simulation methods cannot manage the complex boundaries of a porous medium. The lattice Boltzmann method (LBM) proposed by McNamara and Zanetti (1988) is a mesoscopic simulation method between macroscopic continuous simulation and microscopic molecular dynamics simulation. It is a conventional approach to the problem of porous media seepage (Kruger et al., 2017). LBM can simulate fluid flow and study the influence of particle geometry on the permeability at the pore scale.

Many researchers have used the LBM method to study porous media seepage at the pore scale. Some researchers have used regularly arranged cylinders or balls (Li et al., 2005; Okabe and Blunt, 2004; Shen et al., 2017) whereas others have used various stochastic methods (Lee and Yang, 1997; Maier et al., 1998) to construct a porous medium with simple geometric features to study the seepage law. Particles of natural porous media (soil, sand, sediment, and gravel) cannot be regarded as a regular set of balls and cylinders arranged randomly. Although the porous medium generated by a random method is close to the realistic condition, the influence of the geometric characteristics of the particles on the permeability cannot be studied. Some investigations of the effect of particle shape on the permeability of a porous medium through LBM have been carried out in the past (Stewart et al., 2006; Scholes et al., 2017; Dorai et al., 2012; Saomoto and Katagiri, 2015; Osipovsky, 2017). These studies used regularly shaped particles such as ellipsoids or ellipses and cubes. In reality, natural particles are not of regular shapes. Chukwudozie and Tyagi (2013) examined the effect of the surface characteristics of

particles on the permeability. In their study, the surface characteristics of particles were controlled by means of several bulges above the sphere, and the rule of particle arrangement in the porous medium was periodic body centered cubic, which is very different from the morphological characteristics of real particles. Moreover, the study provides only a qualitative law for the effect of the surface characteristics of particles on the permeability. Some investigations have considered the effect of particle size distribution on the permeability of porous media (Sheikh and Pak, 2015; Yang et al., 2016). Sheikh and Pak (2015) studied the effect of gradation parameters on the permeability by constructing a porous medium using the discrete element method. However, the formula for predicting the permeability coefficient from the gradation parameters could not be derived because of limited calculation conditions. Yang et al. (2016) constructed a porous medium with uniform particle size distribution, and concluded that the randomness of particle arrangement has significant effects on the permeability. However, the number of grids in this study was small and the gradation parameters were not considered. There are also some researches focusing on unsaturated seepage (Dou et al., 2013; Wang et al., 2016, 2019) or rock seepage (Zhang et al., 2016; Akai et al., 2018; Li and Berkowitz, 2018) based on LBM available in literature. However, the morphological characteristics of particle were not considered in unsaturated seepage studies, and the pore structure of rock is very different from that of particle-packed porous medium.

In addition to LBM, some studies have used the finite volume method (FVM) to study the influence of porous media geometry on the permeability at the pore scale (Garcia et al., 2009; Torskaya et al., 2014; Katagiri et al., 2015; Taylor et al., 2017). The disadvantage of these studies is that the general computing conditions are relatively few and only a few qualitative rules can be generated because of the difficulty of FVM modeling. Furthermore, owing to the high computational cost of solving the Navier–Stokes (N-S) equations using the FVM, most of these studies employed calculations based on the Laplace equation instead of the N-S equations.

Most of the above numerical simulation studies only considered one aspect of particle geometry; the calculation conditions were generally relatively limited, and the resulting law was generally qualitative rather than quantitative, which affected its direct application to engineering practice.

Figure 1: Images of sand photographed under the microscope. (a) sand from Plum Island, and (b) Colorado great sand dunes.

What does a real natural particle look like on the pore scale? Greenberg et al. (2015) photographed a series of microscopic images of sand particles across the United States using a three-dimensional microscope. The real pore-scale sand structure is shown in Figure 1. It can be seen that the structure presents more details on the pore scale, such as different size distributions, different shapes, and different surface morphologies. Therefore, to fully consider the influence of particle geometry on the permeability, it is necessary to consider the porosity, particle shape, particle size distribution, and surface characteristics of the particles.

The aim of this paper is to perform a pore-scale simulation of the fluid flow, as shown in Figure 1, and to examine how these geometric properties of the particles affect the permeability of the natural particle-packed porous media such as soil, sand, and gravel. A porous medium with different porosities, shapes, surface features, and particle gradations is considered. LBM is used to study the seepage law at the pore scale and the change in a single variable at a time is strictly ensured, which can overcome the shortcomings of the previous experimental studies. The influence of each geometric factor on the permeability is determined through a large number of numerical simulations under different conditions. In addition, a modified KC formula is presented by considering all geometric factors. The formula is more general than the conventional KC formula and contains parameters that can be easily obtained in engineering.

2. Numerical model

2.1. Numerical model of porous media

In this study, the geometric characteristics of a porous medium are set by controlling the size, number, shape, surface, and size distribution of its particles. The construction of the porous medium is divided into two steps. The particles are constructed first, and then the porous medium is generated on the basis of the constructed particles.

2.1.1. Construction of particles

As shown in Figure 1, sand particles are found to have different particle sizes and shapes when observed under a three-dimensional microscope. Spherical particles are not appropriate for studying the effect of particle morphology on permeability. Two methods for constructing soil particles close to their real shapes are proposed in this paper. The first method is based on the random growth model of cellular automata (CA) (Wang and Pan, 2007) and can be used to construct particles of different shapes; the second method is based on the spherical harmonic function and can be used to construct particles with different surface characteristics.

The basic principle of the CA random growth model is shown in Figure 2. First, a growth center is determined, and then growth occurs randomly along 18 adjacent directions from the growth center at a certain probability. The process of constructing a single soil particle by the CA random growth method can be described as follows:

Step 1: Set the growth probability P_i of each direction according to the desired shape.

Step 2: Each direction grows with probability P_i until the set particle volume is reached.

Step 3: The generated particle surface is operated by a morphological method to make it smooth.

The shape of the particle is controlled by controlling the growth probability in each direction, P_i . When the growth probabilities in the 18 directions are the same, the CA random growth model can generate a particle that is close to a sphere. When the growth probability of the particles is less than 1 in each direction ($P_i < 1$), the surface of the particles will produce a lot of burrs (see Figure 3(a)). Morphological methods were employed in this study to make

Figure 2: CA random growth model.

the surface smooth. The shape of the spherical particles after one morphological close operation and one open operation is shown in Figure 3(b). An ideal sphere is shown in Figure 3(c). Comparing Figures 3(b) and 3(c), it can be seen that the particles generated by the CA random growth model are very close to the sphere, but are more closer to actual soil particles than to the ideal sphere.

Figure 3: Shape of particle constructed by (a) CA random growth model before morphological operation, (b) after morphological operation, and (c) ideal sphere.

Numerous parameters have been proposed to characterize the shape of particles. One of the most commonly used and representative parameter is sphericity. There are several definitions of sphericity; the definition proposed by Wadell (1935) is the most commonly used. The Wadell sphericity can be expressed as

$$S_w = \frac{\sqrt[3]{36\pi V^2}}{S_A}, \quad (2)$$

where V is the volume of the particles and S_A is the surface area of the particles.

Another definition of sphericity was proposed by Kuo et al. (1996). The Kuo sphericity is given as

$$S_k = \sqrt[3]{\frac{d_{\min} d_{\text{med}}}{d_{\max}^2}}, \quad (3)$$

where $d_{\max}$, d_{med} , and $d_{\min}$ are the maximum, middle, and minimum radii of the particles, respectively. It is possible to control the radius in each direction of the particles constructed by the CA random growth model by controlling the growth probability; that is, $d_{\max}$, d_{med} , and $d_{\min}$ can be simply controlled, and then the particles with different Kuo sphericities S_k can be generated. In this study, we used the Kuo sphericity to generate the initial status of the shape of the particles. Then, the accurate surface area of each particle was obtained by the Marching Cubes (MC) method (see section §3.2). The Wadell sphericity, S_w , corresponding to the obtained S_k sphericity can then be calculated. Several particles of different sphericities, produced by the above method, are illustrated in Figure 4.

Figure 4: Particle shapes of different sphericities produced by CA random growth model. (a) $S_w=0.7742$; (b) $S_w=0.8403$; (c) $S_w=0.8712$; and (d) $S_w=0.9121$.

186 The sphericity only represents the shape characteristics of the whole particle and cannot
 187 represent the fluctuation of the particle surface. The fluctuations of the particle surface can
 188 be characterized by roundness or roughness. There are several definitions of roundness, and
 189 the most commonly used definition of roundness was proposed by Cox (1927), which can be
 190 expressed as

$$R_c = \frac{4\pi A}{P^2}, \quad (4)$$

191 where A is the area of the maximum projection of the particles and P is the actual circumference
 192 of the maximum projection. Another parameter that can represent the fluctuation of the particle
 193 surface is the roughness. The definition of particle roughness (Liu and Xia, 2011) is as follows:

$$\sigma_R = \sqrt{\frac{\sum_{i=1}^N \left(\frac{R_i}{\bar{R}}\right)^2}{N}} - 1, \quad (5)$$

194 where R_i is the polar coordinate amplitude of the point on the particle surface, and $\bar{R}$ is the
 195 average value of the polar coordinate amplitude.

196 The spherical harmonic function is used to construct particles of different roundness and
 197 roughness. It has been proven to be a powerful tool for representing the particle morphological
 198 features (Zhou et al., 2015, 2018). Here, the basic concept of the spherical harmonic (SH) theory
 199 is briefly introduced. The polar coordinates of a unit sphere are expanded to the corresponding
 200 polar coordinates of an actual particle by the approximation of the spherical harmonic function
 201 sequence, and the corresponding spherical harmonic coefficients are obtained by the known
 202 polar coordinates set on the particle surface. The real particle surface equations approximated
 203 by the sequence of the spherical harmonic functions are as follows:

$$r(\theta, \varphi) = \sum_{n=0}^{\infty} \sum_{m=-n}^n a_n^m Y_n^m(\theta, \varphi), \quad (6)$$

204 where a_n^m is the spherical harmonic coefficient that needs to be determined. Y_n^m is the spherical
 205 harmonic series, which is given by the following equation:

$$Y_n^m(\theta, \varphi) = \sqrt{\frac{(2n+1)(n-m)!}{4\pi(n+m)!}} P_n^m(\cos \theta) e^{im\varphi}, \quad (7)$$

where P_n^m are the associated Legendre polynomials and n is an integer between 0 and $+\infty$, which is determined by the precision of particle reconstruction. The total number of unknown spherical harmonic coefficients is $(n+1)^2$, which requires $(n+1)^2$ independent equations. To ensure we have sufficient independent equations, we need the polar coordinates of more than $(n+1)^2$ points on the surface of the particle. We can obtain more than $(n+1)^2$ linear equations by substituting this polar coordinate set into (6). Then, the least squares method is used to solve the linear equations to obtain the spherical harmonic coefficients. The equation of the particle surface can be obtained by substituting the spherical harmonic coefficient into (8).

$$\hat{r}(\theta, \varphi) = \sum_{n=0}^{n_{\max}} \sum_{m=-n}^n a_n^m Y_n^m(\theta, \varphi) \quad (8)$$

According to Zhou et al. (2015), the surface roundness and roughness characteristics of the particles can be accurately characterized when $n_{\max}$ is greater than the 15th order. In this study, the 20-order spherical harmonic function is used to construct particles of different roundness and roughness. According to the previous description of the construction method of the spherical harmonic function, polar coordinates of not less than $(20+1)^2 = 441$ points on the surface of the particles are required to calculate the spherical harmonic coefficients. In order to obtain a set of coordinates of not less than 441 points on the surface of particles of different roughness, this paper adopts the method shown in Figure 5 (taking 2D as an example). First, the Fibonacci mesh is used to distribute 1000 points uniformly on a sphere (Richard and James, 2010) of radius R_m , and then the radius at each point is changed by a random method.

$$R_i = R_m + \Delta R \times \text{rand}(-1, 1). \quad (9)$$

Substituting R_i into (5) yields

$$\sigma_R = \frac{\sqrt{3}\Delta R}{3R_m}. \quad (10)$$

It can be concluded from (10) that particles of different roughness can be generated by controlling the size of ΔR while keeping R_m constant. The spherical harmonic coefficient of the spherical harmonic function is obtained by using these 1000 points, and the final equation of the particle surface is obtained by substituting them into (8).

Figure 5: Schematic diagram of (a) Fibonacci grid with spherical uniform distribution points and (b) random generation method for the radius (taking 2D as an example)

The roundness of the particles changes with the change in particle roughness. The outline of the maximum projection plane can be obtained by the bwperim operator in MATLAB, and then the roundness corresponding to the particles of different roughness can be calculated by (4). Several particles of different roughness and roundness, generated by the spherical harmonic method, are shown in Figure 6.

Figure 6: Particles with different surface fluctuations, generated by spherical harmonic method. (a) $R_c=0.9871$; (b) $R_c=0.9360$; (c) $R_c=0.7508$; and (d) $R_c=0.5859$.

2.1.2. Generation of porous medium

The construction of a porous medium is based on the construction of particles by random packing algorithm. Since Kepler's conjecture of sphere packing was proposed in 1611, the

packing problem has been studied for hundreds of years. It is too complex to obtain an accurate solution of hard particle packing because of the jamming phenomenon. The packing of non-spherical particles has received some attention but their characterization is far from complete (Torquato et al., 2000; Torquato and Stillinger, 2010). The existing research on the non-spherical particle packing is mainly focused on ellipsoids (Donev et al., 2004b,a), hypersphere (Yuan et al., 2018), and polyhedrons (Betke and Henk, 2000; Kallus et al., 2010). Although the particle shape is no longer spherical, it can still be regarded as regular geometry. The natural particles are randomly generated under various geological actions and their morphologies are very different from that of regular particles. There is no related algorithm in literature to simulate the packing of natural particles directly.

The packing of irregular particles is investigated in this research. The packing algorithm in this paper fixes the porosity and randomly places the particles in space without overlap; gravity packing is not performed. The process of constructing a porous medium can be described as follows:

Step 1: The calculation grid of the LBM is generated and the number, size, shape, and surface characteristics of the required particles are determined according to the geometric characteristics of the porous medium.

Step 2: The required particle is constructed using the two particle construction methods described in Section §2.1.1.

Step 3: Continuous attempts are made until a random location is found in the mesh where there is no overlap between the generated particles; the particle is placed in that position.

Step 4: Steps 2 and 3 are repeated until the number of particles calculated by Step 1 is reached and the final porous medium is generated.

The position and orientation of the particles is random. Although the porosity of this packing is different from that of gravity packing (in fact, the porosity of the gravity packing is also uncertain owing to the existence of the jamming phenomenon), their geometric characteristics are similar. The purpose of this paper is to study the influence of the geometric characteristics

on the hydraulic characteristics under low Reynolds number. Therefore, the permeability law obtained in this paper can be applied to an actual gravity packed porous medium.

In this study, to examine the influence of different factors, including porosity, shape, surface characteristics, and size distribution, we need to construct multiple porous media with varying factors. This study uses relatively larger numbers of computational lattices (our simulations contain approximately $500 \times 500 \times 500$ lattices). Figure 7 illustrates several typical porous media constructed in the study for each factor.

2.2. Pore-scale numerical modeling of flow

2.2.1. Lattice Boltzmann Method

LBM is a computational fluid dynamics method based on the Boltzmann equation of unbalanced statistical physics and the principle of lattice gas automaton. This method is based on molecular dynamics theory and has a clear physical background. It is a mesoscopic simulation method. LBM simulation is effective for porous media seepage where the traditional computational fluid dynamics method is ineffective.

A complete lattice Boltzmann model usually consists of three parts—the evolution equation of the distribution function, the lattice (velocity discrete model), and the equilibrium distribution function (Kruger et al., 2017). In LBM, the fluid flow is calculated by the discrete Boltzmann equation. The discrete lattice Boltzmann equation without external forces (Chen and Doolen, 1998) can be expressed as follows:

$$f_{\alpha}(\mathbf{r} + \mathbf{e}_{\alpha}\delta_t, t + \delta_t) - f_{\alpha}(\mathbf{r}, t) = -\frac{1}{\tau}[f_{\alpha}(\mathbf{r}, t) - f_{\alpha}^{eq}(\mathbf{r}, t)], \quad (11)$$

where $f_{\alpha}(\mathbf{r}, t)$ denotes the velocity distribution function at time t and at $\mathbf{r}$ position in the α direction, and $f_{\alpha}^{eq}(\mathbf{r}, t)$ is the local equilibrium distribution function. $\mathbf{e}_{\alpha}$ is the discrete velocity in the α direction. δ_t is the time step and τ is the relaxation time. This equation is the evolution equation of the distribution function of the single relaxation LBM.

The discrete velocity model used in this paper is a three-dimensional D3Q19 model proposed by Qian et al. (1992), which is same as the CA random growth model (shown in Fig. 2). The grid velocities in different directions are configured as follows.

Figure 7: Porous medium constructed for each factor. (a) porosity=0.2467; (b) porosity=0.3488; (c) porosity=0.6031; (d) $S_w=0.7742$; (e) $S_w=0.8403$; (f) $S_w=0.9121$; (g) $R_c=0.9360$; (h) $R_c=0.7508$; (i) $R_c=0.4323$; (j) $C_u=2, C_c=1$; (k) $C_u=4, C_c=3$; and (l) $C_u=8, C_c=4$.

$$\mathbf{e}_\alpha = \begin{cases} (0, 0, 0) & \alpha = 0, \\ (\pm 1, 0, 0)c, (0, \pm 1, 0)c, (0, 0, \pm 1)c & \alpha = 1 \sim 6, \\ (0, \pm 1, \pm 1)c, (\pm 1, 0, \pm 1)c, (\pm 1, \pm 1, 0)c & \alpha = 7 \sim 18, \end{cases} \quad (12)$$

where c is the lattice speed obtained as $c = \delta_x/\delta_t$. In the formula, δ_x and δ_t are dimensionless lattice step and time step respectively.

The equilibrium distribution function of the D3Q19 model is

$$f_\alpha^{eq} = \rho \omega_\alpha \left[1 + \frac{\mathbf{e}_\alpha \cdot \mathbf{u}}{c_s^2} + \frac{(\mathbf{e}_\alpha \cdot \mathbf{u})^2}{2c_s^4} - \frac{u^2}{2c_s^2} \right], \quad (13)$$

where c_s is the lattice sound speed ($c_s^2 = c^2/3$) and ω_α is the weight coefficient whose value is as follows:

$$\omega_\alpha = \begin{cases} 1/3 & \alpha = 0, \\ 1/18 & \alpha = 1 \sim 6, \\ 1/36 & \alpha = 7 \sim 18 \end{cases} \quad (14)$$

The above D3Q19 model can be restored to the macroscopic N-S equation by the Chapman-Enskog expansion. The dimensionless relaxation time and the macroscopic kinematic viscosity coefficient ν have the following relationship:

$$\tau = \frac{1}{2} + \frac{\nu}{c_s^2 \delta_t}. \quad (15)$$

The macroscopic density and the macroscopic velocity on each lattice are obtained by the following formulae:

$$\rho = \sum_{\alpha=0}^{18} f_\alpha, \quad (16)$$

$$\mathbf{u} = \frac{1}{\rho} \sum_{\alpha=0}^{18} f_\alpha \mathbf{e}_\alpha. \quad (17)$$

The programming process for the LBM is as follows. Firstly, the local equilibrium function of the lattice point is obtained by using the macroscopic density and velocity. Then, the collision is completed in one time step, following which the velocity distribution function migrates along each lattice velocity direction. After the migration step, the macro velocity and density of the cells are updated and the cycle continues until the flow stabilizes.

2.2.2. Verification of LBM program

A pressure-driven 3D Poiseuille flow is simulated to verify the LBM program. The LBM simulation of a viscous laminar flow does not require a conversion factor. All quantities can be directly considered in dimensionless lattice units, and the final results of the simulation are similar to a dimensional physical flow system with the same Reynolds number owing to the law of similarity.

Figure 8: Illustration of the pipe model (a) and velocity contour in the x direction (b) calculated by LBM.

The Poiseuille pipe model is shown in Figure 8(a). The radius of the pipe (r_p) is 50 and the length (L_p) is 500. The dimensionless relaxation time τ is 1 and the pressure difference (Δp) at both ends of the pipe is $5e - 5$. The pipe wall adopts the standard bounce back scheme, and the entrance and exit adopts the non-equilibrium extrapolation scheme (Guo et al., 2002). The velocity contour calculated by LBM is shown in Figure 8(b) and the maximum velocity $u_{\max} = 3.75e - 4$. The Reynolds number can be obtained as

$$Re = \frac{u_{\max} r_p}{\nu} = 0.225. \quad (18)$$

The theoretical formula for the radial distribution of the Poiseuille flow velocity in a circular tube is

$$u_x(w) = \frac{\Delta p}{4\nu\rho L_p}(r_p^2 - w^2), \quad (19)$$

where w is the distance of any point from the center of the pipe. The comparison between the numerical and analytical solutions of the velocity in the x direction with variation in w is shown in figure 9(a). Compared with the analytical solution, the relative error distribution of the middle cross section of the pipe is shown in figure 9(b). It can be seen that the relative error is small except at the boundary.

Figure 9: Comparison between LBM simulation and theoretical solution of Poiseuille flow (a) and its relative error (b).

The L_2 error norm (Roy, 2005) of the velocity in the x -direction is used to measure the convergence of the calculation. The residual error is calculated every 100 steps, and the formula of the residual error can be expressed as

$$\epsilon_{u_x}(t) = \sqrt{\frac{\sum (u_x(\mathbf{r}, t) - u_x(\mathbf{r}, t - 100\delta_t))^2}{\sum u_x^2(\mathbf{r}, t)}}. \quad (20)$$

The variation of the residual error with the time step is shown in Figure 10. It can be seen that the residual error decreases exponentially with the calculation time step.

The verification of 3D Poiseuille flow shows that the LBM program used in this paper is stable, accurate, and efficient for a flow with low Reynolds number. Therefore, it can be used to simulate a seepage flow with small Reynolds number.

Figure 10: Variation of residual error with time step.

2.3. Numerical model of seepage

In this section, the proposed model is used to simulate the seepage in a porous medium. The schematic diagram of the seepage numerical model is shown in Figure 11. The boundary conditions in the calculation model are set as follows: the non-equilibrium extrapolation scheme of fixed pressure is used for the inflow boundary and the fully developed scheme (Guo et al., 2002) is used for the outflow boundary. The standard bounce back scheme (Lavallée et al., 1991) is used for the other four boundaries and the boundaries of the particles.

τ needs to be greater than 0.5 to satisfy the stability of the numerical calculation (Kruger et al., 2017). τ is set to 1 in this seepage model. As shown in section §2.2.2, the numerical model should be stable, accurate, and efficient. To ensure accuracy, the typical Mach number should not be greater than 0.1 (Feng et al., 2007). The pressure difference driving the seepage is $5e-5$, and the magnitude of maximum velocity of the seepage flow simulated in section §3 is $1e-5$. The typical Mach number of the flow is $1e-5$, which is much less than 0.1. Therefore, the compression error can be completely ignored. Moreover, the typical Reynolds number is $1e-3$, which indicates that the seepage flow is a laminar flow.

The discretization study is applied to spherical particles, particles generated by CA (CA particle), and particles generated by spherical harmonic (SH particle), and the minimum resolution of each particle required for calculation accuracy is determined. At first, three kinds of porous media with random placement of particles are generated by the algorithm in section §2.1. Then, overall scaling is performed to generate porous media with different resolutions. The radius

Figure 11: Schematic diagram of numerical model of seepage.

of a sphere of volume equal to that of each particle is taken as the typical radius (D_t), which can be used to represent the resolution of the particle. The dimensionless permeability under a different resolution is defined as

$$K'_{D_t} = \frac{Kr}{D_t^2}. \quad (21)$$

Pan et al. (2001) and Hilpert (2011) used the Richardson extrapolation to calculate the exact value of the permeability, K'_∞ , when the resolution approaches infinity, which can be expressed as

$$K'_\infty = \frac{(D_{t_2}/D_{t_1})^\lambda K'_{D_{t_2}} - K'_{D_{t_1}}}{(D_{t_2}/D_{t_1})^\lambda - 1}, \quad (22)$$

where λ denotes the order of convergence. In the LBGK model of LBM, $\lambda = 2$ (Kruger et al., 2017). Then, the relative error can be defined as

$$\epsilon(K'_{D_t}) = \frac{|K'_{D_t} - K'_\infty|}{K'_\infty}. \quad (23)$$

The patterns of particles with different resolutions are shown in Figure 12(a). The variation in the relative error of the three particle types with the typical radius is shown in Figure 12(b). It can be seen that the relative error can be controlled within 0.05 when the typical radii of the ball, CA particle, and SH particle are greater than 15, 20, and 25 respectively.

Figure 12: Patterns of particles with different resolutions (a) and the variation of relative error with typical particle radius (b).

A large number of lattices ($500 \times 500 \times 500$) was used in this research to ensure that the resolution of the individual particles meets the above accuracy requirements and that the porous media contains enough particles. We believe that the homogeneity of the randomly generated samples is well satisfied when these many lattices are used because we simulated each of the samples at least twice and found that the results were almost the same.

3. Simulation and analysis

An example of the streamline and velocity field calculated with the present model is shown in Figure 13. It can be seen that the velocity of the fluid and the tortuous flow paths can be easily traced by LBM.

The unit is a dimensionless lattice unit, and the permeability coefficient obtained by Darcy's law is a relative permeability that is proportional to the physical permeability. The formula for calculating the relative permeability can be expressed as follows:

$$Kr = -\frac{\mu \langle u_x \rangle}{\nabla p}, \quad (24)$$

where μ is the lattice viscosity, $\langle u_x \rangle$ is the overall mean value of the velocity in the x direction, and ∇p is the pressure gradient of the calculation model.

Figure 13: (a) Streamlines of flow through non-spherical particles, and velocity contours in (b) the cross section and (c) the longitudinal section.

3.1. Effect of porosity on permeability

To examine the effect of porosity on permeability, it is necessary to ensure that other parameters remain unchanged except the porosity. In this section, the porous media is constructed with smooth spherical particles of the same diameter, which is fixed at 10 lattice unit (lu), and the porosity is controlled by adjusting the number of particles. Particles in a porous medium are randomly arranged. Ten (10) porous media with different porosities varying from 0.2 to 0.8 were constructed (Figure 7) and their permeability was calculated.

The correlation between the permeability coefficient and porosity of the porous medium was determined based on the calculated results of the permeability. According to the KC formula (Eq.1), a linear regression on the relative permeability coefficient Kr and the expression $\phi^3/(1 - \phi)^2$ of the porosity was performed. As shown in the Figure 14, the coefficient of determination R^2 is 0.9891. The relative error between the regression and the calculated values is shown in Figure 14(b). It can be seen that although the overall degree of fitting is high, the relative error is relatively large (nearly 70%) when the porosity is small. The results shown in Figure 15 can be obtained if permeability with porosity less than 0.45 is fitted. At this porosity, the linear correlation between Kr and $\phi^3/(1 - \phi)^2$ remains high but the relative error is much lower although it is still high at 30%. Therefore, the study in this paper shows that the relationship between permeability and porosity in the KC formula is effective, but the relative error is large when the porosity is small.

Figure 14: (a) Linear regression on the relative permeability coefficient Kr and the expression for porosity $\phi^3/(1 - \phi)^2$ and (b) relative error.

Figure 15: (a) Linear regression on Kr and the expression for porosity $\phi^3/(1 - \phi)^2$ when $\phi < 0.45$ and (b) relative error.

Figure 16: Linear regression on the logarithm of Kr and $\phi^3/(1-\phi)^2$.

In order to reduce the relative error caused by low porosity and obtain a suitable correlation between permeability and porosity, the logarithms of Kr and $\phi^3/(1-\phi)^2$ were taken separately and linear regression was performed to obtain the results shown in Figure 16. Here, the coefficient of determination R^2 is 0.9994, which indicates a good degree of fitting, and the problem of large relative error with low porosity is no longer observed. In this case, a new fitting parameter a is introduced on the basis of the KC formula.

$$K \propto \left[\frac{\phi^3}{(1-\phi)^2} \right]^a. \quad (25)$$

With (25), the accuracy of the correlation between the permeability coefficient and the porosity is greatly improved.

Figure 17 shows the linear regression of Kr and $(\phi^3/(1-\phi)^2)^{0.82}$. Compared with Figures 14 & 15, it can be seen that the error is much smaller and the fitting degree has reached 0.9996. Moreover, the relative error of porosity from low to high does not exceed 10%. Therefore, this paper concludes that it is more accurate to replace $\phi^3/(1-\phi)^2$ with $(\phi^3/(1-\phi)^2)^a$ in the KC formula. The parameter a given in this paper is 0.82.

The velocity contours of the longitudinal sections with porosity of 0.2682 and 0.5733 are shown in Figure 18. It can be seen that the seepage channel of the porous medium with small porosity is not obvious, whereas the seepage channel of the medium with large porosity is obvious and a complete seepage network is formed. The velocity of some seepage channels

Figure 17: (a) Linear regression for Kr and $(\phi^3/(1-\phi)^2)^{0.82}$ and (b) relative error.

Figure 18: Velocity contours of longitudinal sections with porosity of 0.2682 (a) and 0.5733 (b).

in the seepage network is obviously greater than that of the other channels; therefore, there is seepage main channel phenomenon in seepage network from pore scale.

For a porous medium with equal particle size, the specific surface area can be obtained as

$$S = \frac{4\pi r^2}{\frac{4}{3}\pi r^3} = \frac{3}{r}. \quad (26)$$

According to the classical KC formula, the relationship between permeability and particle size of a porous medium with equal particle size is $K \propto 1/S^2 \propto r^2$.

Based on the study of porosity, if the particle size is not very different, it can be represented as d . Then, the formula for calculating the permeability coefficient can be modified on the basis of the KC formula as follows:

$$K = C_1 \left[\frac{\phi^3}{(1-\phi)^2} \right]^{0.82} d^2, \quad (27)$$

where C_1 is an empirical constant that needs to be determined by experimental studies.

3.2. Effect of particle shape on permeability

Univariate analysis is commonly used to analyze the effect of particle shape on permeability. Here, the porosity of a porous medium was fixed at 0.6 and 0.45. In order to meet the accuracy requirements, the typical radius of the particle was set to 26.1 ($Dt = 26.1$). The CA random growth method described in Section §2.1.1 was used to construct particles of different sphericities. Then, a porous medium with random rotation and random arrangement of particles was constructed by using the method described in Section §2.1.2. In this paper, the particle shape was measured by Wadell sphericity S_w (Wadell, 1935). Ten porous media with different S_w ranging from 0.77 to 0.92 were constructed for each porosity (Figure 7) and their permeability was calculated. Then, the parameter K'_ϕ was defined as follows to measure the permeability without considering the effect of porosity.

$$K'_\phi = \frac{Kr}{\left[\frac{\phi^3}{(1-\phi)^2} \right]^{0.82}} \quad (28)$$

The calculated results are shown in Figure 19.

Figure 19: Relation between relative permeability coefficient Kr and particle sphericity S_w .

As shown in Figure 19, under constant porosity and other factors, the sphericity increases with increase in the permeability. With the change in sphericity, the rate of change in permeability can reach 20%. Therefore, the effect of sphericity on the permeability is obvious and cannot be ignored. Here, the relationship between permeability and sphericity, which reflects the particle shape characteristics, is directly studied without introducing tortuosity. As shown in Figure 19, it is found through linear regression without intercept that there is a good linear correlation between permeability and sphericity. Therefore, the sphericity S_w can be directly multiplied with the modified KC formula as a parameter.

In addition to analyzing the porous medium generated by the CA random growth model described above, porous media generated by cubes and diamonds are constructed (as shown in Figure 20) and their permeability is calculated. The Wadell sphericity of cube is 0.806 and that of diamond is 0.846. As shown in Figure 19, the permeability of cubes and diamond is approximately 15% lower than that of near-ellipsoidal particles of same sphericity generated by the CA method. Therefore, it can be concluded that when compared with near-ellipsoidal particles with smoother surfaces, the permeability of particles with more obvious edges, such as cubes and diamonds, are smaller. It also shows that sphericity does not fully represent the geometric characteristics of the particles, and the surface characteristics of the particles should also be considered.

The applicability of the KC formula to particles of different shapes was studied in this research. The surface of the porous medium should be extracted by the Digital Image Processing

Figure 20: Seepage channel diagrams of two typical porous media with particle sizes of (a) 10 lu and (b) 35 lu.

(DIP) method to obtain the specific surface area. Several surface recognition algorithms are available in literature, such as voxel counting (Lindquist et al., 1996), two-point correlation functions (Song et al., 2001), adaptive distance gradient filtering (Flin et al., 2005), and marching cubes (MC) (Culligan et al., 2006; McClure et al., 2007). The MC algorithm was employed in this research, as it is more precise (Porter et al., 2010). The result of surface extraction by MC is shown in Figure 21. The specific surface area (S) can be calculated from the result.

The relationship between permeability and $1/S^2$ is shown in Figure 22. It can be seen that the permeability is linearly correlated with $1/S^2$ ($R^2 = 0.6617$), indicating that the classical KC formula (Eq.1) is also applicable to particles of different shapes. Compared with Figure 19, it can be seen that the degree of fitting of S_w is better than that of $1/S^2$. This is because the specific surface area in the traditional KC formula does not contain information about tortuosity, whereas sphericity contains information about tortuosity. As mentioned earlier, sphericity alone does not fully represent the morphological characteristics of the particles. When the sphericity is the same and the roundness is different, the permeability no longer shows a good fit. At this point, the advantages of the classical KC formula appear. It can be seen from the Figure that the specific surface area contains both shape and surface characteristics, and cubic and diamond fit the relationship between permeability and $1/S^2$.

Figure 21: Result of surface extraction by MC.

Figure 22: Relationship between permeability and $1/S^2$ with different particle shapes.

3.3. Effect of particle surface on permeability

The fluctuation of the particle surface can be characterized by roundness or roughness. Univariate analysis was used to analyze the effect of the particle surface on the permeability. As before, parameters other than the surface characteristic parameters of the particles were kept constant. The porosity of the porous medium was fixed at 0.6 and 0.45, and spherical particles of equal diameter were used. According to the method described in Section §2.1.1, the spherical harmonic function was used to construct particles with different roundness (or roughness). It was proved that there is a strict linear negative correlation between roughness and roundness of particles, that is, roundness and roughness are equivalent parameters. The Cox roundness R_c (Cox, 1927) is used to represent the surface characteristics of the particles in the following discussion. Eight porous media with different roundness ranging from 0.43 to 0.99 were constructed with each value of porosity (Figure 7) and their permeability was calculated. The calculation results are shown in Figure 23.

As shown in Figure 23, when the porosity and other factors are kept constant, the permeability increases with increase in the roundness of the particle. With the change in roundness, the rate of change of permeability can reach 60%. Therefore, the effect of roundness on permeability is even more obvious than that of sphericity and cannot be ignored. Here, the relationship between permeability and roundness, which reflects the particle surface characteristics, is directly studied. As shown in Figure 23, it is found through linear regression without intercept that there is a good linear correlation between permeability coefficient and roundness when $R_c > 0.65$. Therefore, the roundness R_c can be directly multiplied with the modified KC formula as a parameter when the roundness is greater than 0.65.

Figure 24 shows the local pore structure and local flow field in the intermediate longitudinal section of a porous medium with particle roundness equal to 0.7742. It can be seen from the pore structure diagram that the particles with roundness equal to 0.7742 are very rough and have many edges. From the local flow velocity contour, it can be seen that the velocity of pores on the rough surface is close to zero. That is, although these pores exist, their contribution to fluid flow is zero. Because of the existence of these ineffective pores on the surfaces of the particles, the effective pores used for fluid flow in the case of rough particles are smaller than the actual pores. The rougher the particle, the smaller is the effective porosity, resulting in smaller permeability.

Figure 23: Relation between Kr and particle roundness R_c .

Figure 24: (a) Local pore structure and (b) local velocity contour in the intermediate longitudinal section of porous medium comprising rough particles.

Figure 25: Relationship between permeability and $1/S^2$ for medium with different particle surfaces.

492 This research examines whether the KC formula is applicable to particles with different
 493 surface characteristics. The MC method is used to obtain the specific surface area and the
 494 relationship between the permeability and $1/S^2$ is shown in Figure 25. It can be seen that the
 495 permeability is linearly correlated with the specific surface area, and a better degree of fitting
 496 than that with R_c is observed ($R^2 = 0.9517$). However, there is an intercept in the linear
 497 relationship, which indicates that the application of the traditional KC formula is also limited
 498 for particles of different roughness. The reason for this is also shown in Figure 24: the effective
 499 surface area and effective porosity change at the same time as the change in roughness. Because
 500 the intercept is not as roundness which is a dimensionless quantity only related to the surface
 501 of the particle, it will change with the particle size distribution. At this point, using the Cox
 502 roundness (R_c) to characterize the surface is advantageous because the threshold roundness is a
 503 definite value ($R_c > 0.65$).

504 3.4. Effect of particle size distribution on permeability

505 The particle size distribution can be characterized by the gradation parameters. There are
 506 three main gradation parameters. The first is the span of the particle size, that is, the ratio of
 507 maximum particle size to the effective particle size, which can expressed as follows.

$$C_r = d_{100}/d_{10} \quad (29)$$

508 The second is the coefficient of non-uniformity, which reflects the distribution of particle groups
509 of different sizes. It is defined as

$$C_u = d_{60}/d_{10}. \quad (30)$$

510 The last is the coefficient of curvature, which is an index that describes the overall shape of the
511 gradation curve. It is defined as

$$C_c = \frac{d_{30}^2}{d_{60}d_{10}}. \quad (31)$$

512 Among these, coefficient of non-uniformity and coefficient of curvature are the most important
513 characteristic gradation parameters. Many experimental studies have been performed on the
514 influence of these two parameters on the permeability. Different studies have reported different
515 effects, including contradicting conclusions (Su et al., 2014; Kong et al., 2011). This is mainly
516 due to the difficulty in controlling various parameters in the experiment. If the soil is well
517 graded, it will inevitably have smaller porosity, which makes it difficult to completely separate
518 these parameters from each other in the experiment. Numerical simulation can solve this prob-
519 lem well. In this paper, the influence of C_u and C_c on the permeability coefficient was studied
520 by LBM numerical simulation.

521 By using the method presented in Section §2.1, different sizes of spherical particles were
522 used to construct porous media with different gradations. In the process of construction, the
523 mean particle size ($d_u = 13.37$ lu) and porosity ($n = 0.6$) were kept constant. The generation
524 method of porous media with soil of different gradations is described below. First, the maximum
525 particle size d_{100} is roughly determined according to the number of particles and porosity. Then,
526 d_{10} is determined by (29) using a given C_r (the span of the particle size C_r is fixed at 10 here).
527 Then, d_{60} is calculated according to (30) using a given C_u , whereas d_{30} is calculated according to
528 (31) using a given C_c . After the above control particle sizes are obtained, the particle size within
529 these control particle sizes is generated randomly by following a uniform distribution. After all
530 particle sizes are determined, the corresponding spherical particles and the porous medium are
531 generated according to the method outlined in Section §2.1. After the first generation, the actual

Figure 26: Gradation curves for different calculation cases.

porosity is calculated based on the total volume of the particles. Based on the ratio of the actual porosity, the particle sizes are magnified or reduced to obtain the final porous medium.

To examine the effect of C_u and C_c on the permeability, fourteen porous media with different gradation parameters were constructed for each porosity (0.45 and 0.6; Figure 7), and their permeability was calculated. The gradation curves for the fourteen porous media are shown in Figure 26.

The relationship between the relative permeability coefficient and the gradation parameters is shown in Figure 27. As shown in the figure, with change in the gradation parameters, the rate of permeability change can reach 120%. Therefore, the effect of particle size distribution on permeability is more obvious than that of particle shape and particle surface characteristics. Figure 27(a) shows that under the same porosity, mean particle size, and other factors, the permeability coefficient increases obviously with increase in the coefficient of non-uniformity. It can be seen from Figure 27(b) that with increase in the coefficient of curvature, the permeability coefficient also increases, but it is not as obvious as the increase in the coefficient of non-uniformity. This implies that the permeability coefficient is more sensitive to the coefficient of non-uniformity.

In this study, the volume and surface area of each particle was calculated and the exact value of the specific surface area of each porous medium was obtained. The relationship between relative permeability and specific surface area is shown in Figure 28. It can be seen from the figure that the permeability coefficient has a good positive correlation with $1/S^2$. This also shows that the KC formula is still fully applicable for particles of different sizes, regardless of the change in gradation.

Figure 27: Relation between relative permeability coefficient and gradation parameters ($\phi = 0.6$). (a) coefficient of non-uniformity and (b) coefficient of curvature.

Figure 28: Relation between relative permeability and specific surface area.

In engineering practice, the specific surface area is a parameter that is not easy to determine. It can be seen from previous studies that the specific surface area is proportional to the square of the particle size when the particle sizes are equal. Therefore, in the case of a medium with unequal particle sizes, it is necessary to find a particle size that can best represent the particle size of the system, which can then be used to replace the specific surface area S in the KC formula. It can be seen from the gradation curve that the variation in d_{10} is very small. Here, we focus on the correlation between the permeability coefficient and d_{30} as well as d_{60} . As shown in Figure 29, the corresponding coefficients of determination are 0.7163 and 0.4114 respectively. In engineering practice, the degree of fit of d_{30} is acceptable. Therefore, d_{30} is suggested as the representative particle size of the particle system. In engineering practice, if the porosity and the control particle size of soil are simply measured, it is suggested that the following prediction formula for the permeability coefficient should be adopted.

$$K = C_2 \left[\frac{\phi^3}{(1 - \phi)^2} \right]^{0.82} d_{30}^2, \quad (32)$$

where C_2 is an empirical constant that needs to be determined by experimental studies. Although (32) is not exactly accurate, it has a certain degree of goodness of fit, which can meet the requirement of an engineering application. It is also consistent with the formula obtained through experiments (Zhu, 2010; Su et al., 2014).

Figure 29: Relation between relative permeability coefficient K_r and control particle sizes. (a) d_{30}^2 and (b) d_{60}^2 .

Figure 30: Relation between relative permeability coefficient K_r and the combination $(C_u + C_c)d_{10}^2$.

Is there a more accurate prediction formula that considers the gradation parameters? In this study, various combinations of gradation parameters and control particle sizes were tested, and the correlation between them and the permeability coefficient was investigated. Finally, it was found that the best linear correlation occurred between the combination $(C_u + C_c)d_{10}^2$ and the permeability coefficient. As shown in Figure 30, the coefficient of determination of linear regression without intercept reaches 0.8883. Therefore, the combination $(C_u + C_c)d_{10}^2$ can be directly multiplied with the KC formula.

Based on the above conclusion, a modified KC formula considering all the geometrical factors of particles is finally presented.

$$K = C \cdot S_w \cdot R_c \left[\frac{\phi^3}{(1 - \phi)^2} \right]^{0.82} (C_u + C_c)d_{10}^2 \quad \text{when } R_c > 0.65, \quad (33)$$

where C is a constant related to the temperature and viscosity of water. It is noted that (33) does not include the specific surface area and tortuosity, which are not easily measured in engineering practice. Instead, the Wadell sphericity S_w , Cox roundness R_c , coefficient of non-uniformity C_u , coefficient of curvature C_c , and the effect particle size d_{10} are used, all of which can be easily obtained in engineering practice.

3.5. multivariate analysis

Multivariate analysis based on real sand particles was used to verify the formula 33. Firstly, some particles of river sand were selected and their 3-D microcosmic images were obtained

Figure 31: 3D μ CT images of scanning specimen and six typical particles.

by μ CT (Figure 31). The morphological characteristics (Wadell sphericity and Cox roundness) of each particle were calculated. Then, porous media with simultaneous changes in multiple factors were generated by the algorithm described in section §2. The patterns of the porous media constructed by the real particles were close to those of a real porous medium (Figure 32).

The relative permeability Kr is calculated according to (33) for all the above-mentioned numerical simulations (at this time, the constant C should be a relative value C_{re} , which is obtained by linear fitting $C_{re}=0.0139$). As shown in Figure 33, regardless of whether univariate or multivariate analysis is adopted, the calculated value of (33) is consistent with the numerical simulation value, and the degree of fitting of the 45° diagonal is 0.9704, which proves that the modified KC formula can accurately predict the permeability.

4. Conclusion

In this study, particles of different shapes were constructed by the CA random growth model, and particles with different surface characteristics were constructed by the spherical harmonic function. Then, porous media with different porosities, different particle sizes, different shapes, different surface features, and different particle size distributions were generated on the basis of the constructed particles. All aspects of the geometric characteristics of real soil were considered. Three-dimensional LBM was used to simulate the seepage flow in porous media at the pore scale. A large number of numerical simulations were performed under different conditions. The key activities and conclusions of this study were as follows.

Figure 32: Porous media constructed by real particles (particle B of Figure 31, $C_u=4$, $C_c=1$).

Figure 33: Relation between numerical value and calculated value by (33) of relative permeability coefficient.

1. The effects of all aspects of the geometric characteristics on the permeability were studied in this paper. It was proven that in addition to the influence of porosity and particle size on the permeability, the influence of particle shape and surface characteristics on the permeability are obvious and cannot be ignored. The sensitivity of various factors to the permeability coefficient in the order of large to small is as follows: porosity>particle size distribution>particle surface>particle shape.
2. Based on the conclusion arrived for each factor, a modified KC formula considering all the geometrical factors was finally provided in (33). The accuracy of the formula was verified. Equation (33) does not include the specific surface area and tortuosity because they are not easily measurable. All the parameters in the modified formula can be easily obtained in engineering practice.
3. Two simple formulae that can be applied to engineering practice were presented. Equation (27) can be used to predict the permeability when the change in the particle sizes of the porous medium is small. When the change in the particle size is relatively large, d_{30} can be used as the representative diameter of the particle system, and the permeability can be predicted by (32). It can be used to arrive at an approximate estimation of the permeability coefficient when using less known parameters in engineering.
4. The following useful conclusions were obtained from the analysis of the seepage flow field at the pore scale. The velocity of some seepage channels in the seepage network is obviously greater than that in other channels, so there is seepage main channel phenomenon in seepage network. Rough particles, have ineffective pores on the surface. The rougher the particle, the smaller is the effective porosity, resulting in smaller permeability.
5. The applicability of the classical KC formula (1) was studied for the case when the geometric characteristics of particles are changed. It was proven that the KC formula is applicable to multi-dispersed spherical particles and non-spherical particles whose surfaces are not very rough. There is limitation of applications for rough surface particles, but the scope of application is not as definite as the modified KC formula (33).

Because all conclusions in this paper are based on LBM numerical simulations, the laws obtained from the analyses are dimensionless. It was determined that C is a constant in the formula, but the specific value has not been provided. This will be investigated in future experimental studies.

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References

- Akai, T., Bijeljic, B., Blunt, M. J., 2018. Wetting boundary condition for the color-gradient lattice boltzmann method: Validation with analytical and experimental data. *Advances in Water Resources* 116, 56–66.
- Alyamani, M. S., Sen, Z., 1993. Determination of hydraulic conductivity from complete grain-size distribution. *Ground Water* 31 (4), 551–555.
- Barr, D. W., 2001. Coefficient of permeability determined by measurable parameters. *Ground Water* 39 (3), 356–361.
- Betke, U., Henk, M., 2000. Densest lattice packings of 3-polytopes. *Computational Geometry* 16 (3), 157–186.
- Beyer, W., 1964. On the determination of hydraulic conductivity of gravels and sands from grain-size distribution. *Wasserwirtschaft Wassertechnik* 14, 165–169.
- Carman, P. C., 1937. Fluid flow through granular beds. *Transactions of the Institution of Chemical Engineers* 15, 150.
- Carman, P. C., 1956. *Flow of Gases Through Porous Media*. Butterworth Scientific Publications.
- Carrier, W. D., 2003. Goodbye, hazen; hello, kozeny-carman. *Journal of Geotechnical and Geoenvironmental Engineering, ASCE* 129 (11), 1054–1056.
- Chapuis, R. P., Aubertin, M., 2003. On the use of the kozenycarman equation to predict the hydraulic conductivity of soils. *Canadian Geotechnical Journal* 40, 616628.
- Chapuis, R. P., Dallaire, V., Marcotte, D., Chouteau, M., Acevedo, N., Gagnon, F., 2005. Evaluating the hydraulic conductivity at three different scales within an unconfined sand aquifer at lachenaie, quebec. *Canadian Geotechnical Journal* 42, 1212–1220.

- Chen, S., Doolen, G. D., 1998. Lattice boltzmann method for fluid flows. *Annual Review of Fluid Mechanics* 30, 329–364.
- Chukwudozie, C., Tyagi, M., 2013. Pore scale inertial flow simulations in 3-d smooth and rough sphere packs using Lattice Boltzmann Method. *AIChE Journal* 59 (12), 4858–4870.
- Collins, R. E., 1976. Flow of fluids through porous materials.
- Cox, E. P., 1927. A method of assigning numerical and percentage values to the degree of roundness of sand grains. *Journal of Paleontology* 1 (3), 179–183.
- Culligan, K., Wildenschild, D., Christensen, B. S. B., Gray, W., Rivers, M., 2006. Pore-scale characteristics of multiphase flow in porous media: a comparison of air–water and oil–water experiments. *Advances in Water Resources* 29 (2), 227–238.
- Donev, A., Cisse, I., Sachs, D., Variano, E. A., Stillinger, F. H., Connelly, R., Torquato, S., Chaikin, P. M., 2004a. Improving the density of jammed disordered packings using ellipsoids. *Science* 303 (5660), 990–993.
- Donev, A., Stillinger, F., Chaikin, P., Torquato, S., 2004b. Unusually dense crystal ellipsoid packings. *Phys Review Letter* 92, 255506.
- Dorai, F., Teixeira, C. M., Rolland, M., Climent, E., Marcoux, M., Wachs, A., 2012. Fully resolved simulations of the flow through a packed bed of cylinders: effect of size distribution. *Chemical Engineering Science* 129, 180–192.
- Dou, Z., Zhou, Z., Sleep, B., 2013. Influence of wettability on interfacial area during immiscible liquid invasion into a 3d self-affine rough fracture: Lattice Boltzmann simulations. *Advances in Water Resources* 61, 1–11.
- Feng, Y., Han, K., Owen, D., 2007. Coupled Lattice Boltzmann Method and discrete element modelling of particle transport in turbulent fluid flows: Computational issues. *International Journal for Numerical Methods in Engineering* 72 (9), 1111–1134.

- 685 Flin, F., Brzoska, J.-B., Coeurjolly, D., Pieritz, R. A., Lesaffre, B., Coleou, C., Lamboley, P.,
686 Teytaud, O., Vignoles, G. L., Delesse, J.-F., 2005. Adaptive estimation of normals and surface
687 area for discrete 3-d objects: application to snow binary data from x-ray tomography. *IEEE*
688 *Transactions on Image Processing* 14 (5), 585–596.
- 689 Garcia, X., Akanji, L. T., Blunt, M. J., Matthai, S. K., Latham, J. P., 2009. Numerical study of
690 the effects of particle shape and polydispersity on permeability. *Physical Review E: Statistical*
691 *Nonlinear and Soft Matter Physics* 80 (1), 021304.
- 692 Greenberg, G., Kiely, C., Clover, K. I., 2015. The secrets of sand: a journey into the amazing
693 microscopic world of sand. Quarto Publishing Group USA Inc.
- 694 Guo, Z. L., Zheng, C. G., Shi, B. C., 2002. Non-equilibrium extrapolation method for velocity
695 and pressure boundary conditions in the lattice boltzmann method. *Chinese Physics* 11 (4),
696 366–374.
- 697 Harleman, D. R. F., Melhorn, P. F., Rumer, R. R., 1963. Dispersion permeability correlation in
698 porous media. *Journal of the Hydraulic Division, ASCE* 893 (2), 67–85.
- 699 Harr, M. E., 2012. *Groundwater and Seepage*. Dover Publications Inc.
- 700 Hazen, A., 1911. Discussion of dams on sand foundation by A.C. Koenig. *Transactions, ASCE*
701 73, 199–203.
- 702 Hilpert, M., 2011. Determination of dimensional flow fields in hydrogeological settings via the
703 mrt Lattice-Boltzmann Method. *Water Resources Research* 47 (9).
- 704 Jabro, J. D., 1992. Estimation of saturated hydraulic conductivity of soils from particle size
705 distribution and bulk density data. *Transactions, ASAE* 35 (2), 557–560.
- 706 Kallus, Y., Elser, V., Gravel, S., 2010. Dense periodic packings of tetrahedra with small repeat-
707 ing units. *Discrete & Computational Geometry* 44 (2), 245–252.
- 708 Katagiri, J., Saomoto, H., Utsuno, M., 2015. Quantitative evaluation of the effect of grain aspect
709 ratio on permeability. *Vadose Zone Journal* 14, 498–502.

- Kaviany, M., 2012. Principles of heat transfer in porous media. Springer Science & Business Media.
- Kong, L. W., Xin-Ming, L. I., Tian, H. N., 2011. Effect of fines content on permeability coefficient of sand and its correlation with state parameters. *Rock and Soil Mechanics* 32, 21–26.
- Kozeny, O. J., 1953. *Das Wasser im Boden. Grundwasserbewegung*. Springer.
- Kruger, T., Kusumaatmaja, H., Kuzmin, A., Shardt, O., Silva, G., Viggien, E. M., 2017. *The Lattice Boltzmann Method: Principles and Practice*. Springer.
- Kuo, C. Y., Frost, J. D., Lai, J. S., Wang, L. B., 1996. Three-dimensional image analysis of aggregate particles from orthogonal projections. *Transportation Research Record Journal of the Transportation Research Board* 1526 (1), 98–103.
- Lavallée, P., Boon, J. P., Noullez, A., 1991. Boundaries in lattice gas flows. *Physica D: Nonlinear Phenomena* 47, 233–240.
- Lee, S. L., Yang, J. H., 1997. Modeling of darcy-forchheimer drag for fluid flow across a bank of circular cylinders. *International Journal of Heat and Mass Transfer* 40 (13), 3149–3155.
- Li, P., Berkowitz, B., 2018. Controls on interactions between resident and infiltrating waters in porous media. *Advances in Water Resources* 121, 304–315.
- Li, Y., LeBoeuf, E. J., Basu, P. K., Mahadevan, S., 2005. Stochastic modeling of the permeability of randomly generated porous media. *Advances in Water Resources* 28, 835–844.
- Lindquist, W. B., Lee, S.-M., Coker, D. A., Jones, K. W., Spanne, P., 1996. Medial axis analysis of void structure in three-dimensional tomographic images of porous media. *Journal of Geophysical Research: Solid Earth* 101 (B4), 8297–8310.
- Liu, Y., Xia, T. D., 2011. Experimental study on influence of particle roughness on shear wave velocity of sand. *Chinese Journal of Geotechnical Engineering* 33 (2), 285–290.
- Maier, R. S., Kroll, D. M., Kutsovsky, Y. E., Davis, H. T., bernard, R. S., 1998. Simulation of flow through bead packs using the Lattice Boltzmann Method. *Physics of Fluids* 10 (1), 60–74.

- McClure, J., Adalsteinsson, D., Pan, C., Gray, W., Miller, C., 2007. Approximation of interfacial properties in multiphase porous medium systems. *Advances in Water Resources* 30 (3), 354–365.
- McNamara, G. R., Zanetti, G., 1988. Use of the boltzmann equation to simulate lattice gas automata. *Physical Review Letters* 61, 2332–2335.
- Okabe, H., Blunt, M. J., 2004. Prediction of permeability for porous media reconstructed using multiple-point statistics. *Physical Review E* 70, 066135–1–066135–10.
- Onur, E. M., Shakoor, A., 2015. Relationships between grain size distribution indexes and permeability of sands. *Engineering Geology for Society and Territory* 3, 287–290.
- Osiptsov, A. A., 2017. Hydraulic fracture conductivity: effects of rod-shaped proppant from Lattice-Boltzmann simulations and lab tests. *Advances in Water Resources* 104, 293–303.
- Pan, C., Hilpert, M., Miller, C. T., 2001. Pore-scale modeling of saturated permeabilities in random sphere packings. *Physical Review E* 64 (6), 066702.
- Porter, M. L., Wildenschild, D., Grant, G., Gerhard, J. I., 2010. Measurement and prediction of the relationship between capillary pressure, saturation, and interfacial area in a napl-water-glass bead system. *Water Resources Research* 46 (8).
- Qian, Y. H., DHumüres, D., Lallemand, P., 1992. Lattice bgk models for navier-stokes equation. *Europhysics Letters* 17, 479484.
- Richard, S., James, P. R., 2010. Fibonacci grids: a novel approach to global modelling. *Quarterly Journal of the Royal Meteorological Society* 132 (619), 1769–1793.
- Rosas, J., Lopez, O., Missimer, T. M., Coulibaly, K. M., Dehwah, A. H., Sesler, K., Lujan, L. R., Mantilla, D., 2014. Determination of hydraulic conductivity from grain-size distribution for different depositional environments. *Groundwater* 52 (3), 399–413.
- Roy, C. J., 2005. Review of code and solution verification procedures for computational simulation. *Journal of Computational Physics* 205 (1), 131–156.

- 761 Saomoto, H., Katagiri, J., 2015. Particle shape effects on hydraulic and electric tortuosities: a
 762 novel empirical tortuosity model based on van genuchten-type function. *Transport in Porous*
 763 *Media* 107 (3), 781–798.
- 764 Scheidegger, A. E., 1958. The physics of flow through porous media. University Of Toronto
 765 Press: London.
- 766 Scholes, O. N., Clayton, S. A., Hoadley, A. F. A., Tiu, C., 2017. Permeability anisotropy due to
 767 consolidation of compressible porous media. *Transport in Porous Media* 68 (3), 365–387.
- 768 Seelheim, F., 1880. Methoden zur bestimmung der durchlässigkeit des bodens. *Analytical and*
 769 *Bioanalytical Chemistry* 19 (1), 387–418.
- 770 Sheikh, B., Pak, A., 2015. Numerical investigation of the effects of porosity and tortuosity
 771 on soil permeability using coupled three-dimensional discrete-element method and lattice
 772 boltzmann method. *Physical Review E Statistical Nonlinear and Soft Matter Physics* 91 (5),
 773 053301.
- 774 Shen, L. F., Wang, Z. L., Li, S. J., 2017. Numerical simulation for seepage field of soil based on
 775 mesoscopic structure reconfiguration technology. *Rock and Soil Mechanics* 11, 3307–3314.
- 776 Song, S.-R., Jones, K. W., Lindquist, B. W., Dowd, B. A., Sahagian, D. L., 2001. Synchrotron
 777 x-ray computed microtomography: studies on vesiculated basaltic rocks. *Bulletin of Vol-*
 778 *canology* 63 (4), 252–263.
- 779 Stewart, M. L., Ward, A. L., Rector, D. R., 2006. A study of pore geometry effects on anisotropy
 780 in hydraulic permeability using the lattice-boltzmann method. *Advances in Water Resources*
 781 29 (9), 1328–1340.
- 782 Su, L. J., Zhang, Y. J., Wang, T. X., 2014. Investigation on permeability of sands with different
 783 particle sizes. *Rock and Soil Mechanics* 35 (5), 1289–1294.
- 784 Taylor, H. F., O’Sullivan, C., Sim, W. W., Carr, S. J., 2017. Sub-particle-scale investigation of
 785 seepage in sands. *Soils and Foundations* 57 (3), 439–452.

- 786 Terzaghi, K., Peck, R. B., Mesri, G., 1996. Soil Mechanics in Engineering Practice. John Wiley
787 & Sons Inc.
- 788 Torquato, S., Stillinger, F. H., 2010. Jammed hard-particle packings: From kepler to bernal and
789 beyond. *Reviews of Modern Physics* 82 (3), 2633.
- 790 Torquato, S., Truskett, T. M., Debenedetti, P. G., 2000. Is random close packing of spheres well
791 defined? *Physical Review Letters* 84 (10), 2064.
- 792 Torskaya, T., Shabro, V., Torres-Verín, C., Salazar-Tio, R., Revil, A., 2014. Grain shape effects
793 on permeability, formation factor, and capillary pressure from pore-scale modeling. *Transport*
794 *in Porous Media* 1020 (1), 71–90.
- 795 Vukovic, M., Soro, A., 1992. Determination of Hydraulic Conductivity of Porous Media from
796 Grain-Size Composition. Water Resources Publications.
- 797 Wadell, H., 1935. Volume, shape, and roundness of quartz particles. *Journal of Geology* 43 (3),
798 250–280.
- 799 Wang, M., Chen, Y.-F., Ma, G.-W., Zhou, J.-Q., Zhou, C.-B., 2016. Influence of surface rough-
800 ness on nonlinear flow behaviors in 3d self-affine rough fractures: Lattice Boltzmann simu-
801 lations. *Advances in water resources* 96, 373–388.
- 802 Wang, M., Pan, N., 2007. Numerical analyses of effective dielectric constant of multiphase
803 microporous media. *Journal of applied physics* 101 (11), 114102.
- 804 Wang, Y., Chung, T., Armstrong, R. T., McClure, J. E., Mostaghimi, P., 2019. Computations
805 of permeability of large rock images by dual grid domain decomposition. *Advances in Water*
806 *Resources* 126, 1–14.
- 807 Yang, P., Wen, Z., Dou, R., Liu, X. L., 2016. Permeability in multi-sized structures of ran-
808 dom packed porous media using three-dimensional lattice boltzmann method. *International*
809 *Journal of Heat and Mass Transfer* 1064, 1368–1375.

- 810 Yuan, Y., Liu, L., Zhuang, Y., Jin, W., Li, S., 2018. Coupling effects of particle size and shape
811 on improving the density of disordered polydisperse packings. *Physical Review E* 98 (4),
812 042903.
- 813 Zhang, D., Papadikis, K., Gu, S., 2016. A lattice boltzmann study on the impact of the geo-
814 metrical properties of porous media on the steady state relative permeabilities on two-phase
815 immiscible flows. *Advances in Water Resources* 95, 61–79.
- 816 Zhou, B., Wang, J., Wang, H., 2018. Three-dimensional sphericity, roundness and fractal di-
817 mension of sand particles. *Géotechnique* 68 (1), 118–30.
- 818 Zhou, B., Wang, J., Zhao, B., 2015. Micromorphology characterization and reconstruction of
819 sand particles using micro x-ray tomography and spherical harmonics. *Engineering Geology*
820 184 (14), 126–137.
- 821 Zhu, C. H., 2010. Damming the soil properties of water conservancy projects. Ph.D. thesis,
822 Northwest Agriculture and Forestry University.

Highlights

- CA random growth model is used to construct particles with different shapes and spherical harmonic function is used to construct particles with different surface characteristics.
- All aspects of the geometric characteristics of soil are considered and their influence law on permeability is given.
- A modified formula of KC formula considering all geometrical factors is given which is more accurate and parameters in it are easy to be obtained in engineering

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