Simulation of the relationship between porosity and tortuosity in porous media with cubic particles*

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Tortuosity is an important parameter used in areas such as vascular medicine, neurobiology, and the field of soil permeability and diffusion to express the mass transport in porous media. It is a function of the porosity and the shape and distribution of particles. In this paper, the tortuosity of cubic particles is calculated. With the assumption that the porous medium is homogeneous, the problem is converted to the micro-level over a unit cell, and geometry models of flow paths are proposed. In three-dimensional (3D) cells, the flow paths are too complicated to define. Hence, the 3D models are converted to two-dimensional (2D) models to simplify the calculation process. It is noticed that the path in the 2D model is shorter than that in the 3D model. As a result, triangular particles and the interaction are also taken into consideration to account for the longer distance respectively. We have proposed quadrate particle and interaction (QI) and quadrate and triangular particle (QT) models with cubic particles. Both models have shown good agreement with the experimental data. It is also found that they can predict the toruosities of some kinds of porous media, like freshwater sediment and Negev chalk.

Keywords: tortuosity, porosity, porous media, cubic particles

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1. Introduction

Tortuosity is of fundamental importance in the fields of flow, diffusion, and conductance, because many definitions and parameters are related to this concept. In a porous system, the presence of solid particles causes the actual paths of species to deviate significantly from the straight lines.

Normally, the tortuosity is defined as[1−3]

$$\tau = \frac{L_e}{L}, \tag{1}$$

where L_e and L are the actual length of the flow path and the straight length or thickness of the sample along the macroscopic pressure gradient direction, respectively. While some other researchers define the tortuosity as the square of τ in Eq. (1). In the work, equation (1) is used for the definition. Although the definition of tortuosity is straightforward, it is very difficult to determine the actual paths that the ions or molecules travel, because the paths in porous materials are very complicated.

Efforts are made to estimate the tortuosity by experimental, empirical, and theoretical approaches. Two experimental methods are used to estimate the tortuosity. One method measures the diffusion coefficients of the chosen non-reactive species in both free solution and sediment of known porosity,[4] but this method will take weeks or even months. The other method measures the formation factor, which is obtained by the measurements of electrical resistivity, but the experiment requires specialized equipments.

The empirical approaches involve the use of adjustable parameters to fit the experimental data. However, those adjustable parameters vary significantly for different materials and different pore geometries. Hence, many empirical relationships between porosity and tortuosity have been developed.[4−6]

The theoretical methods are based on a specific model of porous medium.[7−9] These methods do not contain any adjustable parameters. Many models are developed, because porous materials have different tortuosities even when they have the same porosity.

The cube is one of the most basic shapes, because it has straight edges, then the calculations are relatively simple. The relationships between poros-

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ity and tortuosity for cubic particles were studied by Comitti and Renaud,[10] Koponen *et al.*,[11,12] and Yu and Li.[13] Comiti and Renaud conducted experiments on the flow through beds packed with spherical and cubic particles, and the model gave

$$\tau = 1 + P\ln(1/\phi). \tag{2}$$

Wyllie and Gregory[14] obtained the value of P experimentally using the fluid flow through unconsolidated porous aggregates, and for cubic particles, they found $P = 0.63$.

Koponen *et al.*[11] applied the lattice-gas cellular-automaton method to solve numerically the creeping flow of a Newtonian incompressible fluid in a two-dimensional (2D) porous medium of randomly placed rectangles of equal size, the model gave

$$\tau = 1 + 0.8(1 - \phi). \tag{3}$$

Konponen *et al.*[12] considered the conception of percolation threshold ϕ_c and modified the above model to give

$$\tau = 1 + a\frac{(1-\phi)}{(\phi - \phi_c)^m}, \tag{4}$$

where $a = 0.65$, $m = 0.19$, and $\phi_c = 0.33$. The porosity varied in the range from 0.40 to 0.90.

Yu and Li[13] proposed a simple geometry model and used 2D square particles to determine the tortuosity of the flow path in a porous medium. Both overlapped and non-overlapped particles were taken into consideration. The model gave

$$\tau = \frac{1}{2}\left[1 + \frac{1}{2}\sqrt{1-\phi} + \sqrt{1-\phi}\cdot\frac{\sqrt{\left(1/\sqrt{1-\phi}-1\right)^2 + 1/4}}{1-\sqrt{1-\phi}}\right]. \tag{5}$$

However, the selected paths could not ensure the required periodicity, and the cell chosen could not ensure the homogeneity of the porous medium.

Recently, Matyka *et al.*[14] used a numerical method (the lattice Boltzmann method) to solve the flow equations in the low Reynolds number regime, found the flow streamlines, and then determined the tortuosity of the flow with cubic particles. The result they obtained is closely related to Eq. (2).

Pisani[15] simulated a diffusion process by using a numerical method and expressed the tortuosity with the porosity and the shape factor, the procedure was simple. When the density of the solid objects was low, the tortuosity of cubic particles was

$$\tau = [1 - 0.73(1-\phi)]^{-1}. \tag{6}$$

However, the process to obtain both models mentioned above is complicated, and numerical technologies and related academic concepts are necessary. In this framework, the geometry method is performed. The general idea is the derivation of a macroscopic behavior from the description at the micro-level that refers to the phenomena over a representative elementary volume (REV). Representative paths are selected to ensure the rationality and the periodicity of the models. Predictive models are functions of porosity and have no empirical parameter. Finally, the reliability and the applications of the proposed models are verified. Although the procedure of getting the model is not as rigorous as those in the above models,[14,15] it is simpler and may lead to similar results.

2. Models of 3D and 2D unit cells

2.1. Calculation models from 3D to 2D

The tortuosity is considered in a porous medium with two-dimensional quadrate particles. Two assumptions are used. The porous medium is homogeneous. The solid part is non-deformable and impermeable.

This work focuses on a simple expression of the moving paths. In this paper, 3D cubic models are converted to 2D models of quadrate particles. As shown in Fig. 1, the path $AOED$ used in the 2D model is the shortest one of all. Therefore, the other cells, which can take the place of longer distance, should be selected with cell A to simulate the tortuosity of the 3D

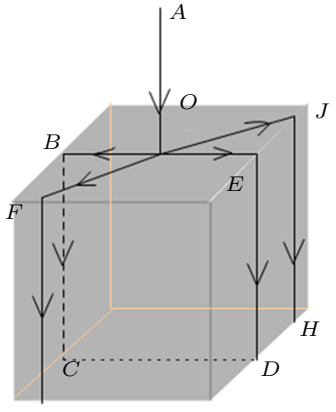


Fig. 1. 3D model.

cubic particles. The interaction and triangular particles are chosen. For the quadrate particle and interaction (QI) model, the interaction is considered to replace the longer distance, while for the quadrate and triangular particle (QT) model, another basic shape of the particle is chosen to replace the longer distance. Both models are described in Fig. 2. Cells A and B are selected in the QI model, and cells A and C are selected in the QT model, as shown in Fig. 2.

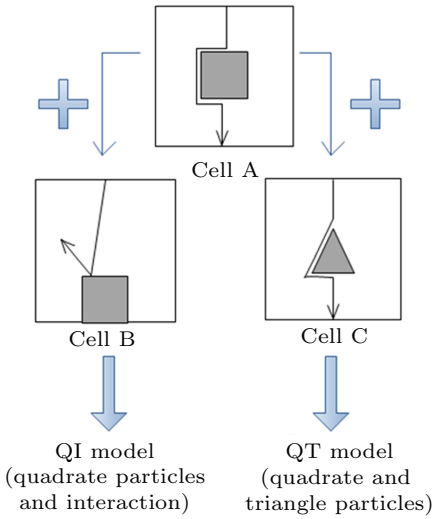


Fig. 2. 2D Model.

2.2. QI model

In this work, a geometric method is applied by averaging over possible lines around the particles to determine the tortuosity. Figures 3(a) and 3(b) show unit cells A and B for quadrate particles. As shown, the lengths of the unit cell and the particle are $(a+b)$ and b, respectively. When the interaction occurs, the paths of the left and the middle points are as shown in Figs. 4(a) and 4(b), respectively. When the interaction does not occur, the lines and the ions move along the edges of the particles, as shown in Fig. 4(c).

The average tortuosity in the porous medium with cubic particles can be obtained using the model of interaction as

$$\tau_{\mathrm{QI}} = \frac{3}{4} + \frac{1}{8}\sqrt{1+\frac{1}{4}\frac{1-\phi}{2-\phi-2\sqrt{1-\phi}}} + \frac{1}{8}\sqrt{1+\frac{1-\phi}{2-\phi-2\sqrt{1-\phi}}} + \frac{1}{4}\sqrt{1-\phi}. \tag{7}$$

The derivation of Eq. (7) is shown in Appendix A. The above equation indicates that when $\phi \to 1$, $\tau_i \to 1$ and when $\phi \to 0$, $\tau_i \to \infty$, both of which are consistent with the physical situation.

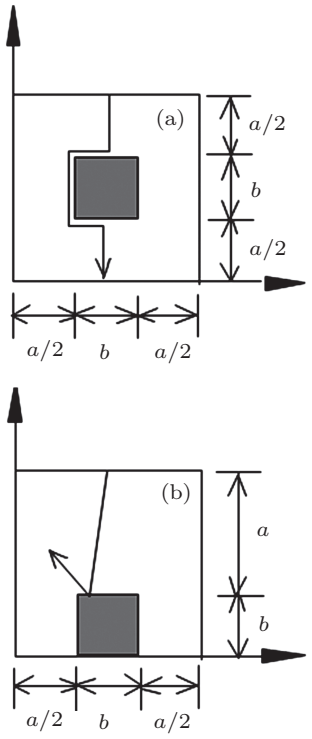


Fig. 3. (a) Unit cell A in the QI model and (b) unit cell B in the QI model.

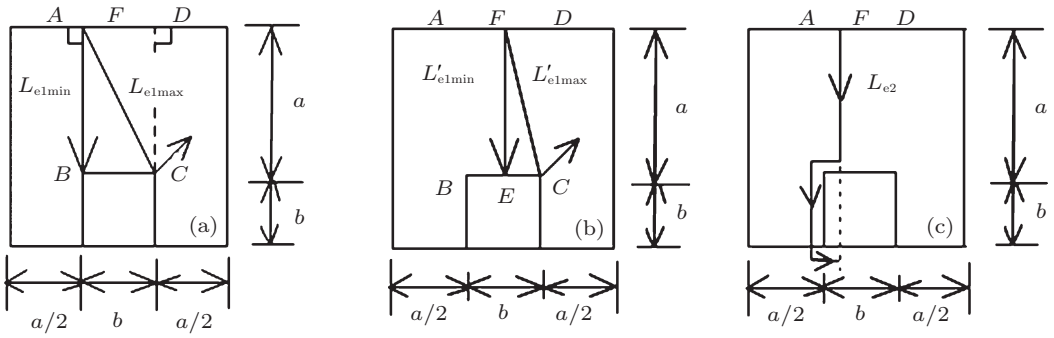


Fig. 4. (a) Paths of point A (when interaction occurs), (b) paths of point F (when interaction occurs), (c) paths of points from A to F (when interaction does not occur).

2.3. QT model

Figures 5(a) and 5(b) show the unit cells for the triangular particles. As shown, the lengths of the unit cell and the edge of the triangle particle are $(a+b)$ and b, respectively. Figure 6 shows the paths when the particles are quadrate and triangular, respectively.

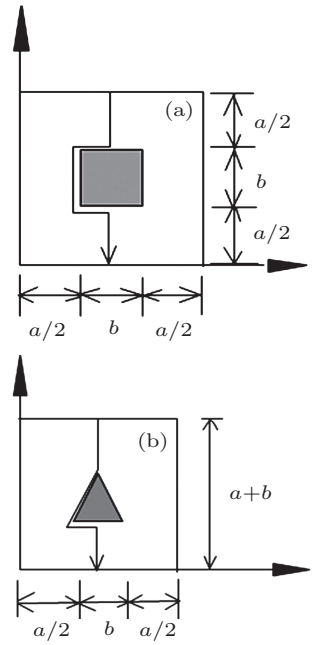


Fig. 5. (a) Unit cell A in the QT model, and (b) unit cell C in the QT model.

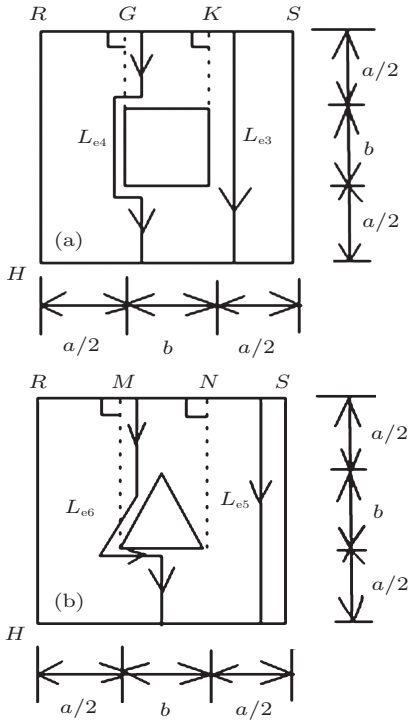


Fig. 6. (a) Paths of cell A in the QT model (when the particle is square), and (b) paths of cell C in the QT model (when the particle is triangle).

The average tortuosity in the porous medium with cubic particles can be obtained using the QT model as

$$\tau_{\mathrm{QT}} = 1 + \frac{\sqrt{1-\phi}}{4\left(2/\sqrt{1-\phi}-1\right)} + \frac{\left(1-\sqrt{3}/4\right)\sqrt{1-\phi}}{\sqrt[4]{3}\left(\sqrt[4]{3}/\sqrt{1-\phi}-1\right)}. \quad (8)$$

The derivation of Eq. (8) is provided in Appendix B. The above equation indicates that when $\phi \to 1$, $\tau_t \to 1$ and when $\phi \to 0$, $\tau_t \to \infty$, both of which are consistent with the physical situation.

3. Discussion

The QI and QT models are developed to calculate the tortuosity of the porous medium with cubic particles. In Fig. 7, the results are compared when the porosity is large. The figure shows that the QI and QT models are in good agreement with the predictions of the other models and the available data for the porous medium with cubic particles. For the QI model, the difference is less than 5% except when the porosity is near 1.0. Although the QI and QT models are developed by using different methods and paths, they are in good agreement over a wide range of porosities. Relatively significant differences are observed only when the porosity approaches 0.8 or is less than 0.45. For the other conditions, the values provided by the QI model are larger than those provided by the QT model. Figure 8 shows the comparison of the results produced by the present two models and the experimental data obtained for different shapes. In the experiment (Wyllie and Gregory), materials of different shapes are made of glass. When the porosity is the same, the tortuosity of the cubic particles is maximum, and the tortuosity of the spherical particles

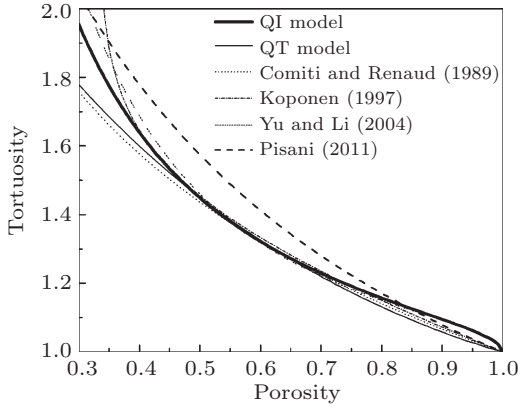


Fig. 7. Comparison among different models.

is minimum. Figure 8 shows that the QT model has better agreement with the experimental data obtained with cubic particles than the QI model.

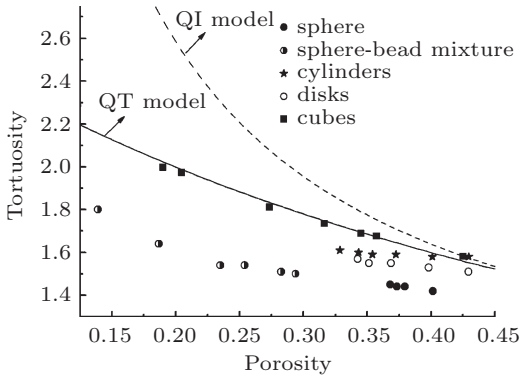


Fig. 8. Comparison among the two models and the experimental data of different shapes of particles (Wyllie and Gregory, 1955).

In addition, it is possible to use the present models to predict the torosities of different soils. As shown in Fig. 9, τ–ϕ data sets are created by combining data of the diffusion of sulfate and methane in marine sediments, the molecular diffusion in freshwater sediments, the gas diffusion in a medium made of dry kaolinite, sand, and celite, and the consolidated chalk from the Negev desert.[4,16−20] It is obvious that except for some data for sand, the QI and QT models provide the primary trends in these data, even the data come from different soils and solutes. When the porosity is larger than 0.65, values obtained by both models are at their lowest limits. When the porosity is between 0.2 and 0.6, the QI and QT models provide a reasonably robust representation of the mean behavior of natural fine-grained porous media. The QI and QT models could predict the toruosities of some kinds of porous media, like freshwater sediment and Negev chalk.

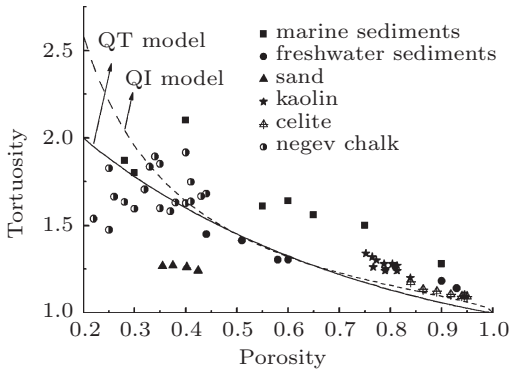


Fig. 9. Comparison between the two models and the experimental data of different kinds of soils.

The method in this paper may be used to simulate the tortuosity. Because the assumption includes that the porous medium is homogeneous, the shape of sphere may be considered similarly. Related lines are similar with those in Fig. 4. Representative values of length need to be calculated and averaged to achieve the new model. However, for the shapes of cylinder and the mixtures, the method in this paper seems not so effective because of their inhomogeneity. The shape of cylinder can be seen as a square and a circular from vertical and horizontal directions, so the anisotropy should be considered. The mixtures are even more complicated. These will be analyzed in depth in our future work.

4. Conclusions

(i) The tortuosity of porous medium depends on the porosity, the granule shape and size distribution, and the saturation. It can be noticed that particles of different shapes may simulate different kinds of porous media. The cube is one of the most basic shapes of particles. With cubic particles, we present two 2D models to simulate the relationship between tortuosity and porosity in three-dimensional porous media based on the REV. The results from the proposed QI and QT models are functions of porosity without empirical constant. In this paper, the geometry method is used, which makes the simulation process much simpler. And similar methods can be used to simulate the tortuosity of particles of some other shapes in the future work.

(ii) The QI and QT models are in good agreement with the related models and experimental data studying the relationship between tortuosity and porosity with cubic particles. When the porosity is between 0.45 and 0.8, the results produced by the QI and QT models are almost identical. For the other conditions, the values provided by the QI model are larger than those provided by the QT model.

(iii) When materials have the same porosity, the tortuosity of the porous medium with cubic particles is maximum.

(iv) The QI and QT models are acceptable predictors for the tortuosity in the porous medium with artificial cubic particles, and they can also provide a prediction of the mean trend for a combined data set

of different natural porous media. What is more, the QI and QT models can predict the toruosities of some kinds of porous media, like freshwater sediment and Negev chalk.

Appendix A

As shown in Fig. 3(a), the lengths of the unit cell and the particle are $(a+b)$ and b, respectively. Hence the total area of the unit cell is $A_t = (a+b)^2$, and the total pore area in the unit cell is $A_p = (a+b)^2 - b^2$. Therefore, for unit cell A or B, the porosity of the cell is given by

$$\phi = 1 - \frac{b^2}{(a+b)^2}. \tag{A1}$$

The above equation can be transformed to

$$\frac{a}{b} = \frac{1}{\sqrt{1-\phi}} - 1. \tag{A2}$$

Figures 4(a) and 4(b) show the paths of the left and the middle points when the interaction occurs. Half of the solid particle is chosen because the cell is symmetrical. A random point on line AD is considered to make sure that the interaction between the ion and the particle can occur. The point moves in the vertical direction. When the interaction occurs, the point collides on the edge of the BC and travels in another direction. The straight length of interaction L_1 is defined as

$$L_1 = a. \tag{A3}$$

When the point is A, the maximum and the minimum lengths from point A to edge BC are, respectively,

$$L_{\mathrm{e1\,max}} = \sqrt{a^2+b^2}, \tag{A4}$$

$$L_{\mathrm{e1\,min}} = a. \tag{A5}$$

The average value L_{e1} is chosen as the actual moving length from point A to edge BC

$$\begin{aligned} L_{\mathrm{e1}} &= \frac{1}{2}(L_{\mathrm{e1\,max}} + L_{\mathrm{e1\,min}}) \\ &= \frac{1}{2}(\sqrt{a^2+b^2} + a). \end{aligned} \tag{A6}$$

When point F is in the middle of AD, the maximum, the minimum, and the actual lengths from F to edge BC are, respectively,

$$L'_{\mathrm{e1\,max}} = \sqrt{a^2 + (\frac{b}{2})^2}, \tag{A7}$$

$$L'_{\mathrm{e1\,min}} = a, \tag{A8}$$

$$\begin{aligned} L'_{\mathrm{e1}} &= \frac{1}{2}(L'_{\mathrm{e1\,max}} + L'_{\mathrm{e1\,min}}) \\ &= \frac{1}{2}\left(\sqrt{a^2 + \left(\frac{b}{2}\right)^2} + a\right). \end{aligned} \tag{A9}$$

The value of distance from all points to edge BC is replaced by the average value of the actual moving lengths from points A and F to edge BC. Hence, when the interaction occurs, the tortuosity is defined as

$$\begin{aligned} \tau_1 &= \frac{(L_{\mathrm{e1}} + L'_{\mathrm{e1}})}{2L} \\ &= \frac{2a + \sqrt{a^2+b^2} + \sqrt{a^2 + (b/2)^2}}{4a}. \end{aligned} \tag{A10}$$

Substituting Eq. (A2) into the above equation, we obtain

$$\begin{aligned} \tau_1 = \frac{1}{2} &+ \frac{1}{4}\sqrt{1 + \frac{1}{4}\frac{1-\phi}{2-\phi-2\sqrt{1-\phi}}} \\ &+ \frac{1}{4}\sqrt{1 + \frac{1-\phi}{2-\phi-2\sqrt{1-\phi}}}. \end{aligned} \tag{A11}$$

When the interaction does not occur, the point moves along the edge of the particle, as shown in Fig. 4(c). Because the periodicity must be ensured, the ending point of the path should be at the position of the initial point of the next periodic cell. Therefore, if the start point is in the middle of AD, the maximum length is

$$L_{\mathrm{e2\,max}} = a + 2b. \tag{A12}$$

If the start point is A, the minimum length is

$$L_{\mathrm{e2\,min}} = a + b. \tag{A13}$$

As the start point moves from A to the middle of edge AD, the actual path varies linearly. Therefore, when the interaction does not occur, the average value of maximum and minimum tortuosities is defined as

$$\begin{aligned} \tau_2 &= \frac{(L_{\mathrm{e2\,max}} + L_{\mathrm{e2\,min}})}{2L} \\ &= \frac{2a+3b}{2(a+b)} \\ &= 1 + \frac{1}{2}\sqrt{1-\phi}. \end{aligned} \tag{A14}$$

In the QI model, the tortuosity is defined by combining the occurrence and the non-occurrence of interaction, i.e., Eq. (7)

$$\begin{aligned}\tau_{\rm QI} &= \frac{1}{2}(\tau_1+\tau_2)\\ &= \frac{3}{4}+\frac{1}{8}\sqrt{1+\frac{1}{4}\frac{1-\phi}{2-\phi-2\sqrt{1-\phi}}}\\ &\quad+\frac{1}{8}\sqrt{1+\frac{1-\phi}{2-\phi-2\sqrt{1-\phi}}}\\ &\quad+\frac{1}{4}\sqrt{1-\phi}. \end{aligned} \tag{A15}$$

Appendix B

The lengths of the unit cell and the edge of the triangular particle are $(a+b)$ and b, respectively, as shown in Fig. 5. The relationship between porosity and the length of the edge of the particle is the same as that in the QI model. As a result, all points move in one direction and travel along the edge of the particle until they reach the bottom. The vertical direction is selected. Half of the particle is chosen to consider the actual length of the path to avoid the existence of repetitive paths. Paths are shown in Figs. 4(a) and 4(b).

When the solid is quadrate, two cases exist. When the start point is between points R and G, it moves in a straight vertical direction without reaching the particle. In this case, the tortuosity is

$$\tau_3 = 1. \tag{B1}$$

When the point is between points G and K, half of the cell is considered. If the starting point is G, the actual moving length is the minimum

$$L_{\rm e4\,min} = a+b. \tag{B2}$$

As the point moves to the middle of the edge of GK, the actual moving length $L_{\rm e4}$ increases linearly to the maximum

$$L_{\rm e4\,max} = a+2b. \tag{B3}$$

Hence, the average value of the minimum and the maximum lengths is selected to calculate the tortuosity when the point is between GK

$$L_4 = \frac{1}{2}(L_{\rm e4\,min}+L_{\rm e4\,max}) = a+\frac{3}{2}b, \tag{B4}$$

$$\tau_4 = \frac{2a+3b}{2(a+b)}. \tag{B5}$$

According to the distribution of the length and half of the particle, the weighted factor is taken into consideration

$$\begin{aligned}\tau'_{\rm B} &= \frac{2a}{2a+b}\cdot\tau_3+\frac{b}{2a+b}\cdot\tau_4\\ &= 1+\frac{1}{2/\sqrt{1-\phi}(2/\sqrt{1-\phi}-1)}. \end{aligned} \tag{B6}$$

When the particle is triangular, all points in cell C move and end at the middle of the edge of the bottom of the triangular particle to express the very long distance. The porosity of cell C is

$$\phi = 1-\frac{\sqrt{3}b^2}{4(a+b)^2}. \tag{B7}$$

The formula can be transformed to

$$\frac{a}{b} = \frac{\sqrt[4]{3}}{2\sqrt{1-\phi}}-1. \tag{B8}$$

When the starting point is between points R and M, it moves in a straight vertical direction without reaching the particle. In this case, the tortuosity is

$$\tau_5 = 1. \tag{B9}$$

When the starting point is M, the minimum length occurs

$$L_{\rm e6\,min} = a+b+\frac{b}{2} = a+\frac{3}{2}b. \tag{B10}$$

As it moves to the middle of MN, the actual length of L_6 increases linearly to its maximum

$$\begin{aligned}L_{\rm e6\,max} &= \left(a+b-\frac{\sqrt{3}}{2}b\right)+b+\frac{b}{2}\\ &= a+\left(\frac{5-\sqrt{3}}{2}\right)b. \end{aligned} \tag{B11}$$

Hence, the average value of the minimum and the maximum lengths is selected to calculate the tortuosity when the start point is between MN

$$\begin{aligned}L_{\rm e6} &= \frac{1}{2}(L_{\rm e6\,min}+L_{\rm e6\,max})\\ &= a+\left(\frac{8-\sqrt{3}}{4}\right)b, \end{aligned} \tag{B12}$$

$$\tau_6 = \frac{a+((8-\sqrt{3})/4)b}{a+b}. \tag{B13}$$

Then the weighted factor is taken into considera-

tion

$$\tau''_{\mathrm{B}} = \frac{2a}{2a+b}\cdot\tau_5 + \frac{b}{2a+b}\cdot\tau_6 = 1 + \frac{2-\sqrt{3}/2}{\sqrt[4]{3}/\sqrt{1-\phi}(\sqrt[4]{3}/\sqrt{1-\phi}-1)}. \quad \text{(B14)}$$

In the QT model, the tortuosity is defined when the particles can be both quadrate and triangular, which is Eq. (8)

$$\tau_{\mathrm{QT}} = \frac{1}{2}(\tau'_{\mathrm{B}} + \tau_{\mathrm{B}}'') = 1 + \frac{1}{2}\frac{1}{2/\sqrt{1-\phi}(2/\sqrt{1-\phi}-1)} + \frac{1}{2}\frac{2-\sqrt{3}/2}{\sqrt[4]{3}/\sqrt{1-\phi}(\sqrt[4]{3}/\sqrt{1-\phi}-1)}. \quad \text{(B15)}$$

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