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Construction of a model for calculating average tortuosity of porous media based on optimal fractal structure

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Abstract: The distribution of pores and skeletons in porous media materials are irregular, and its distribution of curved pore channels is uneven and complex. The bending degree of pores affects the internal heat transfer process. The tortuosity is not only a parameter to describe the bending degree of pore channels, but also is one of the important structural basic parameters of porous media materials. According to the porosity of the porous media materials, Sierpinski carpet model is established to characterize its structures. The calculation model of the average tortuosity of the porous media materials is derived by using the average value of the route of the heat flow through Sierpinski carpet. In order to find the best fractal unit structure and the number of iterations in the average tortuosity calculation model, an optimization discriminant model is established. The results of the average tortuosity calculation model of this model and the other three scholars are compared, and their average relative errors are calculated to be all less than 1 %, indicating that the average tortuosity calculation model established in this study is effective and reliable. The average tortuosity prediction model is related to the fractal unit structure and stage of the carpet, and there is no empirical constant in this model. It can be used to calculate the average tortuosity of other porous media materials, providing a new idea for calculating the average tortuosity.

Keywords: Average tortuosity; Sierpinski carpet; Porous media materials; Heat flow paths.

1. Introduction

Porous media materials with solid phase as the solid skeleton, with gas or liquid or gas-liquid two-phase for the pore structure, and its pore structure is interconnected and complex. When studying the permeability, electrical conductivity and thermal conductivity of porous media materials, it is necessary to consider the macroscopic transport properties of porous media in their microstructure [1-3].

For example, in the study of thermal conductivity of porous media materials, in addition to porosity affects the heat transfer inside the porous media materials, the bending degree of the pores also affects the heat transfer process inside the porous media materials. Because of the irregular distribution of pores and skeletons in porous media materials, the distribution of curved pore channels is uneven and complex. Therefore, the tortuosity is not only a parameter to describe the bending degree of pore channels, but also is one of the important structural basic parameters of porous media materials [4]. Moreover, tortuosity is also widely used in energy conversion and storage systems such as oil exploitation, carbon sequestration, fuel cells, and lithium-ion batteries. It is also used as an effective geometric parameter to describe ion transport in porous material electrodes [5-6] and an important parameter index for designing fixed bed reactors [4].

At present, the methods of calculating tortuosity are experimental measurement, numerical simulation and theoretical analysis. Numerical simulation methods are random walk numerical simulation [7-8,15], corrugated pore structure model (CPSM) [9-11], maximum sphere method [12], lattice gas simulation method (LG) [13], FLUENT numerical simulation [4], etc. These methods don't require too much theoretical basis and they can be calculated by software. However, these methods usually have one or more empirical constants and some errors, and the calculation process is complex. In order to make the calculation simple, some scholars use the theoretical analysis model to calculate. Such as Lanfrey et al. [16] derives the theoretical model of the tortuosity of the random filling of the same spherical particles, which can be used to calculate the tortuosity of porous media materials with porosity between 0.36 and 0.45. However, when calculating materials with low porosity or high porosity, the experimental error is large. Some scholars have also studied the microstructure of porous media materials based on fractal theory. For example, Yuan Pei et al. [14] bases on the accurate self-similar Sierpinski carpet model, which can be used to calculate the tortuosity of porous media materials with porosity between 0.75-1. Similarly, Du et al. [4] obtains the relationship between tortuosity and porosity by changing the geometric shape of the regular polygon solid matrix in the Sierpinski carpet. The results are not much different from the FLUENT numerical simulation results. However, when the number of regular polygon edges increases, the tortuosity does not change much, and only the tortuosity of porous media materials with porosity below 0.9 can be calculated. However, the above scholars are based on the Sierpinski carpet with a fractal unit of 3×3 to establish the tortuosity calculation model, which is not friendly to the calculation of the tortuosity of porous media materials with high porosity. Porous media materials with different porosity can be characterized by different fractal unit structures. So finding the best fractal unit structure is what this paper needs to consider.

Basing on the previous theoretical research and considering the porosity of porous media is different. Since Sierpinski carpet is used to characterize its internal microstructure, its fractal unit structure should not be static. Therefore, in order to calculate the average tortuosity of aerogels or porous media materials suitable for various porosities, this paper is based on the average tortuosity calculation model of Sierpinski carpet with self-similar 3×3 of LI Jianhua et al. [17]. The average tortuosity calculation model of Sierpinski carpet with fractal unit structure of $k\times k$ is derived. The optimal fractal unit structure and stage of porous media materials are found to determine the average tortuosity calculation model. This study provides a new idea for calculating the average tortuosity of porous media materials with high porosity.

2. Establish an average tortuosity model

2.1. Sierpinski carpet fractal process of different fractal units

Since the internal pores of porous media materials are disordered and complex, Sierpinski carpet can be used to simulate it. Changing the fractal unit structure of Sierpinski carpet can better characterize its internal structure. At present, the most basic Sierpinski carpet is composed of 3×3 fractal unit structure. However, since the Sierpinski carpet with fractal unit structure of 3×3 is not suitable for characterizing porous media materials with high porosity, its maximum porosity is only 0.8889. In order to find the average tortuosity calculation model suitable for porous media materials with high porosity, this paper further extends the Sierpinski carpet based on 3×3 fractal unit structure. And we are used to the Sierpinski carpet composed of $k\times k$ fractal unit structure to characterize porous media materials. Moreover, because of the diversity of Sierpinski carpets composed of even fractal units, this paper only considers Sierpinski carpets composed of odd fractal units. When $k>1$ is a positive integer and odd, the Sierpinski carpet with the fractal unit structure $k\times k$ starts as a square with a side length of 1. In the first iteration, a square with a side length of $1/k$ is removed from the center of the square with a side length of 1. In the second iteration, the remaining k^2-1 sub-square shapes with a side length of $1/k$ are removed from their central $(1/k)^2$ sub-squares as in the first iteration. Therefore, the schematic diagram of the Sierpinski carpet with the fractal unit structure $k\times k$ is as follows. The black area represents the solid phase (porous material skeleton) area, and the blank area represents the gas phase (pore) area.

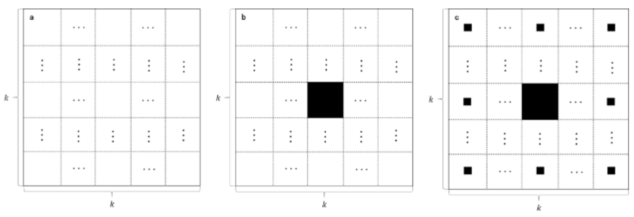

Fig. 1 Sierpinski carpet with fractal unit of $k\times k$.

Figure 1 (a) is the basic fractal unit fractal, Figure 1 (b) is the fractal unit after the first iteration, and Figure 1 (c) is the fractal unit after the second iteration.

2.2. Calculation of average tortuosity based on heat flow paths

The tortuosity τ_i is defined as:

$$\tau_i=\frac{L_{ei}}{L_i} \tag{1}$$

where L_{ei} is the true length of the curved pore channel; L_i is the linear length at both ends of the curved pore channel.

The average tortuosity τ is defined as:

$$\tau=\frac{\sum_{i=1}^{N}\tau_i}{N} \tag{2}$$

where, N is the number of connected curved pore channels.

The average tortuosity is closely related to the fractal dimension or porosity of the material [11-13]. In this paper, the Sierpinski carpet with a fractal unit of $k\times k$ is constructed by the porosity of the porous medium material, and then the Sierpinski carpet with a fractal unit of $k\times k$ is used to construct the average tortuosity model. The Schematic of heat flow paths is as follows:

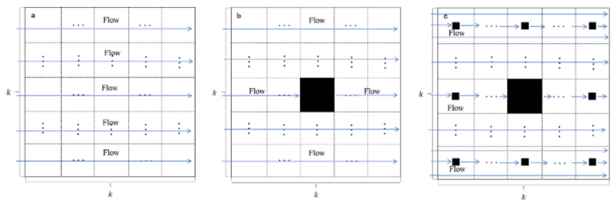

Fig. 2 Schematic of heat flow paths of Sierpinski carpet with fractal unit of $k\times k$.

Fig.2 (a) is a zeroth-stage Sierpinski carpet with a fractal unit of $k\times k$, whose heat conduction direction is set from left to right, and the actual length of the curved pore channel is equaled to the length of the straight line at both ends of the linked curved pore channel, then its average tortuosity is $\tau(0)=1$. Fig.2 (b) is a 1st-stage Sierpinski carpet with a fractal unit of $k\times k$, whose heat flow line has twists and turns in the middle sub-square, and the law of heat flow line needs to be further analyzed at this position. Fig.2 (c) is a 2nd-stage Sierpinski carpet with a fractal unit of $k\times k$, whose streamline has twists and turns in multiple sub-squares, and its formation process needs to be deduced according to the 1st-stage Sierpinski carpet.

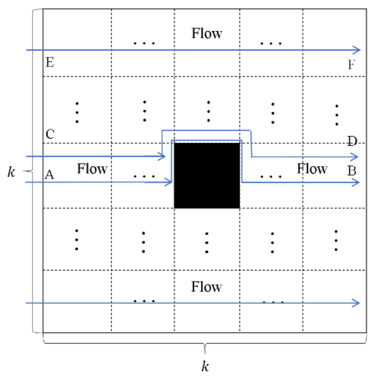

Fig. 3 Schematic of flow paths through the 1st-stage Sierpinski carpet with fractal unit of $k\times k$.

Figure 3 is the 1st-stage Sierpinski carpet 's Schematic of heat flow paths. By simulating its streamline, we are found that the heat flow diagram can be divided into k parts from top to bottom. That is a row of squares to be a part. Except for part $(k+1)/2$, the remaining pore channels are approximately straight. And the average tortuosity of this part $k-1$ is

$$\tau_1 = \tau_2 = \cdots = \tau_{\frac{k+1}{2}-1} = \tau_{\frac{k+1}{2}+1} = \cdots = \tau_k = \frac{\sum_{i=1}^{N} 1}{N} = 1 \tag{3}$$

The tortuosity of part $(k+1)/2$ is more complex. Among them, the flow path of $A \rightarrow B$ is the longest, and the average tortuosity is

$$\tau_{\frac{k+1}{2}}^{A\rightarrow B} = \frac{L_{e\frac{k+1}{2}}}{L_{\frac{k+1}{2}}} = \frac{1+\frac{1}{2k}\times 2}{1} = \frac{k+1}{k} \tag{4}$$

The streamline of $C \rightarrow D$ is approximately 1. Therefore, the average tortuosity of part $(k+1)/2$ takes the longest and shortest averages as

$$\tau_{\frac{k+1}{2}} = \frac{\frac{k+1}{k}+1}{2} = \frac{2k+1}{2k} \tag{5}$$

Therefore, the average tortuosity of the 1st-stage Sierpinski carpet with a fractal unit of $k \times k$ is

$$\tau(1) = \frac{\frac{2k+1}{2k}+k-1}{k} = \frac{2k^2+1}{2k^2} \tag{6}$$

Since the average tortuosity of zeroth-stage Sierpinski carpet with a fractal unit of $k \times k$ is $\tau(0)=1$, the average tortuosity of the 1st-stage Sierpinski carpet with a fractal unit of $k \times k$ can be rewritten as

$$\tau(1) = \frac{2k^2+1}{2k^2}\tau(0) \tag{7}$$

where $\tau(0)$ represent the average tortuosity of the zeroth-stage Sierpinski carpet with a fractal unit of $k \times k$, and $\tau(1)$ represent the average tortuosity of the 1st-stage Sierpinski carpet with a fractal unit of $k \times k$.

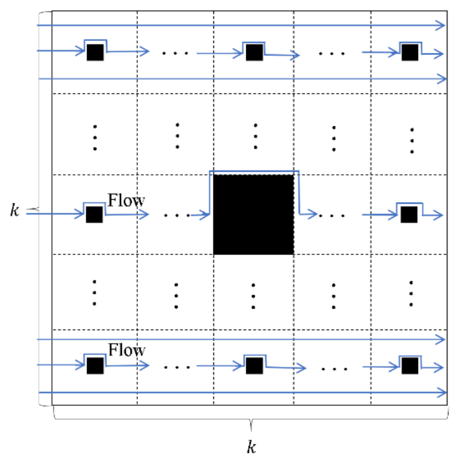

Fig. 4 Schematic of flow paths through the 2nd-stage Sierpinski carpet with fractal unit of $k \times k$.

Figure 4 is the 2nd-stage Sierpinski carpet 's Schematic of heat flow paths. By simulating its streamline, the k^2 sub-square is divided into k^2 parts. It is found that except for the $[(k+1)/2]th$ sub-square, the average tortuosity of the other k^2-1 sub-square is $1/k$ of the 1st-stage Sierpinski carpet. That is

$$\tau_1 = \cdots = \tau_{\frac{k^2+1}{2}-1} = \tau_{\frac{k^2+1}{2}+1} = \cdots = \tau_{k^2} = \frac{1}{k}\tau(1) \tag{8}$$

the average tortuosity of the $[(k+1)/2]th$ sub-square is

$$\tau_{\frac{k+1}{2}} = \frac{\frac{1}{2k}\times 2+\frac{1}{k}+\frac{1}{k}}{2}\tau(1) = \frac{3}{2k}\tau(1) \tag{9}$$

The 2nd-stage Sierpinski carpet with a fractal unit of $k \times k$ is then divided into k parts from top to bottom. Excepting for part $(k+1)/2$. The average tortuosity of the other $k-1$ parts is

$$\tau^1 = \tau^2 = \cdots = \tau^{\frac{k+1}{2}-1} = \tau^{\frac{k+1}{2}+1} = \cdots = \tau^k = k \times \frac{1}{k}\tau(1) = \tau(1) \tag{10}$$

Since the average tortuosity of the $[(k+1)/2]th$ part of the 2nd-stage Sierpinski carpet is similar to that of the 1st-stage Sierpinski carpet. The average tortuosity of this part is

$$\tau^{\frac{k+1}{2}} = \frac{3}{2k}\tau(1) + (k-1)\times\frac{1}{k}\tau(1) = \frac{2k+1}{2k}\tau(1) \tag{11}$$

Therefore, the average tortuosity of the 2nd-stage Sierpinski carpet with a fractal unit of $k \times k$ is

$$\tau(2) = \frac{\frac{2k+1}{2k}\tau(1)+(k-1)\tau(1)}{k} = \frac{2k^2+1}{2k^2}\tau(1) \tag{12}$$

Where $\tau(1)$ represent the average tortuosity of the 1st-stage Sierpinski carpet with a fractal unit of $k \times k$, and $\tau(2)$ represent the average tortuosity of the 2nd-stage Sierpinski carpet with a fractal unit of $k \times k$.

By Eq. (7) and Eq. (12), and so on, the average tortuosity of the 1st-stage Sierpinski carpet is

$$\tau(n+1) = \frac{2k^2+1}{2k^2}\tau(n) \tag{13}$$

where $n = 0,1,2,\cdots$. represent the stages of the Sierpinski carpet with a fractal unit of $k \times k$.

Moreover, since $\tau(0)=1$, the average tortuosity model of Sierpinski carpet with a fractal unit of $k \times k$ can also be written as

$$\tau(n) = \frac{2k^2+1}{2k^2}\tau(n-1) = (\frac{2k^2+1}{2k^2})^2\tau(n-2) = \cdots = (\frac{2k^2+1}{2k^2})^n\tau(0) = (\frac{2k^2+1}{2k^2})^n \tag{14}$$

where $k>1$ is a positive integer and is odd, n is a positive integer and $\tau(n)$ is the average tortuosity of the nth- stage Sierpinski carpet with a fractal unit of $k \times k$.

2.3. Optimization of the best fractal unit structure

The porosity of porous media materials can be used to construct Sierpinski carpet. And in turn, Sierpinski carpet can also be used to characterize the internal microstructure of porous media materials. When the porosity of Sierpinski carpet is closer to the porosity of porous media materials, the characterization effect is better. Therefore, we are found the best fractal unit structure by the difference between the porosity after Sierpinski carpet iteration and the real porosity. When the difference between them is smaller, the internal structure of the porous media material is not only better, the average tortuosity calculated by the model is but also more accurate. The true porosity of porous media materials is set to ϕ_0 . In the 1st-stage Sierpinski carpet with a fractal unit of $k \times k$, since the solid phase portion accounts for $1/k^2$, its porosity is:

$$\phi_1 = 1 - \frac{1}{k^2} = \frac{k^2 - 1}{k^2} \tag{15}$$

After n iterations, the porosity of Sierpinski carpet is:

$$\phi_n = (\frac{k^2 - 1}{k^2})^n \tag{16}$$

The difference between the true porosity of the porous media material and the porosity of the Sierpinski carpet iteration is set to be t, which is defined as:

$$t = \phi_0 - \phi_n = \phi_0 - (\frac{k^2 - 1}{k^2})^n \tag{17}$$

where $k > 1$ is a positive integer and odd, n is a positive integer, ϕ_0 is the true porosity of the porous media material and ϕ_n is the porosity of the nth- stage Sierpinski carpet with a fractal unit of $k \times k$.

Here, the dimension (k) and the number of iterations (n) of the optimal fractal unit structure are obtained by establishing an optimization model:

$$\min t = \phi_0 - (\frac{k^2 - 1}{k^2})^n \tag{18}$$

$$s.t. \begin{cases} k > 1 \text{ is a positive integer and is odd}, \\ n \geq 1 \text{ is a positive integer}, \\ \phi_0 > (\frac{k^2 - 1}{k^2})^n 。\end{cases} \tag{19}$$

From the optimization model, k and n can be obtained and the average tortuosity can be calculated.

2.4. Verification of the average tortuosity calculation model

The validity of the model is tested according to the three more accurate models in the current average tortuosity study. Koponen [13] is used the Lattice Gas Simulation (LG) method to calculate the average tortuosity of low Reynolds number flows in a two-dimensional matrix formed by randomly placed fully overlapped rectangles. The formula is

$$\tau_K = 0.8(1 - \phi) + 1 \tag{20}$$

where 0.8 is the fitting constant, ϕ is the porosity of porous media, and τ_K is the average tortuosity of porous media.

Comparing it with the results of the average tortuosity calculation model established in this paper, the relative error is

$$error_{\tau_K} = \frac{|\tau - \tau_K|}{\tau} \times 100\% \tag{21}$$

Yuan Pei et al. [14] are derived the average tortuosity calculation model by n iterations of the self-similar Sierpinski carpet model:

$$\tau_{YP} = \frac{3}{2} - \frac{1}{2}\phi \tag{22}$$

where 0.8 is the fitting constant, ϕ is the porosity of porous media, and τ_{YP} is the average tortuosity of porous media.

Comparing it with the results of the average tortuosity calculation model established in this paper, the relative error is

$$error_{\tau_{YP}} = \frac{|\tau - \tau_{YP}|}{\tau} \times 100\% \tag{23}$$

Du Peng et al. [4] are summarized the relationship between tortuosity and porosity in Sierpinski carpets at low Reynolds numbers as:

$$\tau_{DP} = 1 - (1 - \sqrt{2})(1 - \phi) \tag{24}$$

where 0.8 is the fitting constant, ϕ is the porosity of porous media, and τ_{DP} is the average tortuosity of porous media.

Comparing it with the results of the average tortuosity calculation model established in this paper, the relative error is

$$error_{\tau_{DP}} = \frac{|\tau - \tau_{DP}|}{\tau} \times 100\% \tag{25}$$

Therefore, the validity of the average tortuosity calculation model established in this paper can be tested by observing the size of $error_{\tau_K}$, $error_{\tau_{YP}}$ and $error_{\tau_{DP}}$. In this paper, when the three relative errors are less than 0.1 %, the average tortuosity calculation model of porous media materials is effective.

3. Application and test of the average tortuosity model

3.1. Application of the average tortuosity model

In this paper, five aramid nanofiber aerogels (ANFAs) samples were selected. The preparation method was used KOH / DMSO to deprotonate aramid fibers to obtain aramid nanofiber dispersions, and then was used water to reduce their structures. Finally, aramid nanofiber aerogels were obtained. The fractal dimensions at different magnifications are close, and ANFAs is statistical self-similarity [18]. According to the porosity of 5 samples, the number of iterations of Sierpinski carpet with 10 different fractal unit structures can be calculated respectively. The following table shows:

This paper expects to use small dimension fractal unit structure to characterize porous media materials in the case of small error. Taking sample 1 as an example, the difference between its true porosity and the porosity of Sierpinski carpet with fractal unit structure of 21×21 is only 0.002039. And the relative error is 0.21 %, which can well characterize the internal microstructure of ANFAs. Therefore, this paper only lists the Sierpinski carpet data of 10 fractal unit structures, without considering the higher-dimensional fractal unit structure.

Table 1. The number of iterations of 5 samples under Sierpinski carpets with different fractal structures

sample number	ϕ_0	The number of iterations of Sierpinski carpet with different fractal unit structures									
		3×3	5×5	7×7	9×9	11×11	13×13	15×15	17×17	19×19	21×21
1	99.0752%	1	1	1	1	2	2	3	3	4	5
2	99.057%	1	1	1	1	2	2	3	3	4	5
3	99.0509%	1	1	1	1	2	2	3	3	4	5
4	98.9372%	1	1	1	1	2	2	3	4	4	5
5	98.7793%	1	1	1	1	2	3	3	4	5	6

By Eq. (18) and Eq. (19), the best fractal unit structures of the five samples are 17×17, 17×17, 17×17, 19×19, 9×9, and the number of iterations are 3, 3, 3, 4, 1, respectively. According to Eq. (14), the average tortuosity of the five samples under the Sierpinski carpet of the corresponding fractal unit structure can be calculated. The results are shown in Table 2:

Table 2. The average tortuosity calculation results of 5 samples

sample number	ϕ_0	$k\times k$	n	$\tau(n)$
1	99.0752%	17×17	3	1.005199
2	99.057%	17×17	3	1.005199
3	99.0509%	17×17	3	1.005199
4	98.9372%	19×19	4	1.005552
5	98.7793%	9×9	1	1.006173

According to Table 2, when the porosity is larger, the average tortuosity is gradually reduced in general case. However, if the porosity gap is below 0.03 %, the average tortuosity remains unchanged.

3.2. Model validation

The average tortuosity calculated based on Table 2 is compared with the average tortuosity calculation model established by Koponen, Yuan Pei, Du Peng and others. From the Eq. (21), Eq. (23) and (25), it can be obtained:

Table 3. Comparison of calculated results between this model and other tortuosity prediction models

sample number	ϕ_0	the average tortuosity			
		τ_K	τ_{YP}	τ_{DP}	$\tau(n)$
1	99.0752%	1.0073984	1.004624	1.003831	1.005199
2	99.057%	1.007544	1.004715	1.003906	1.005199
3	99.0509%	1.0075928	1.0047455	1.003931	1.005199
4	98.9372%	1.0085024	1.005314	1.004402	1.005552
5	98.7793%	1.0097656	1.0061035	1.005056	1.006173

According to the comparison of the results of the tortuosity prediction model in this paper with the other three prediction models, it is found that their average relative errors are 0.2674 %, 0.0362 % and 0.1234 % respectively. Therefore, the average tortuosity calculation model in this paper is effective and reliable. Moreover, it can be used to calculate the tortuosity of high porosity materials such as aerogels. The model in this paper is only related to the fractal unit structure of Sierpinski carpet and the number of iterations. It not only has no empirical constant, but also can be used as a new method to calculate the average tortuosity.

4. Conclusions

According to the porosity of the porous media materials, Sierpinski carpet model was established to characterize its structures. The calculation model of the average tortuosity of the porous media materials was derived by using the average value of the route of the heat flow through Sierpinski carpet. In order to find the best fractal unit structure and the number of iterations in the average tortuosity calculation model, an optimization discriminant model is established.

According to the data of 5 samples, the results of the average tortuosity calculation model of this model and the other three scholars are compared, and their average relative errors are calculated to be 0.2674 %, 0.0362 % and 0.1234 % respectively, indicating that the average tortuosity calculation model established in this study is effective and reliable.

The average tortuosity prediction model established in this paper has no empirical constant, which reduces the subjective error of model calculation. It can be used to calculate the average tortuosity of other porous media materials, providing a new idea for calculating the average tortuosity.

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