Construction of the Aerogel Thermal Conductivity Model based on $k \times k$ Sierpinski Carpet Fractal Units

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Abstract: With the characteristics of low density, high specific surface area, and high porosity, aerogel boasts prominent advantages in the field of thermal protection. The thermal insulation performance of aerogel has a significant relationship with its internal microstructure. In this study, the thermal conduction model of Sierpinski aerogel filled with solid in gas is established based on the equivalent circuit method. We calculated the optimal fractal unit structure of the aerogel via its porosity, applied it to the thermal conductivity calculation of four types of aerogels, and revealed the average relative error of less than 11.58%, which is lower than the calculation results of the thermal conductivity model of the aerogel with the fractal unit structure of $3 \times 3$, indicating the effectiveness and reliability of the proposed thermal conductivity prediction model.

Keywords: Thermal conductivity model, optimal fractal unit structure; Sierpinski carpet model; aerogel.

1. Introduction

The intensification of energy consumption and excessive global CO2 emissions have become global concerns in recent years, the importance of energy management and energy consumption reduction has increased[1]. Using insulation materials to reduce heat flow for insulation can effectively improve energy efficiency[2]. For example, insulation materials can be applied in space environments with large temperature differences, playing a crucial role in human safety and stable equipment operation[3]. Moreover, insulation materials are widely used in our daily lives, including firefighting, diving, steelmaking, polar, and exploration[4]. In the past decade, aerogel, with its high porosity, small pore size and correspondingly low thermal conductivity, has proven to be an ideal thermal insulation material.

Currently, researchers have established various calculation methods for the thermal conductivity of aerogels. First, the thermal conductivity is calculated through the heat transfer theoretical model. The heat transfer of aerogel is divided into three modes, namely, convection heat transfer, solid conduction heat transfer, and radiation heat transfer. The thermal conductivity of aerogel in air is approximately the sum of gas phase heat transfer (λgas), skeleton (λsolid), and radiation (λrad)[5], denoted as $λ_{eff} = λ_g + λ_s + λ_r$, whose advantage is considering many factors, such as porosity, specific surface area, density, and temperature. However, errors may exist in the experimental measurement values of each parameter, resulting in inaccurate calculation of thermal conductivity[6-9]. In addition to these parameters, some factors cannot be measured by experimental instruments, such as the specific extinction coefficient of aerogel, the mean free path of gas molecules, and the average group velocity of phonons, which greatly limit the application fields of these heat conduction models[6-9]. Second, the thermal conductivity of aerogel is obtained using numerical simulation methods, including lattice Boltzmann method (LBM)[10-14], coupled finite volume method (FVM)[10,11], direct simulation Monte Carlo (DSMC)[10,14], and molecular dynamics (MD)[10]. The advantage of this method is the simplicity of the empirical correlation and the accuracy of the calculation results, in terms of the narrowness of the scope of application, the rigmarole of computer calculation time, and the large demand for experimental data. Moreover, due to the complex structure and heat transfer process of aerogel materials, the overall heat transfer characteristics of aerogel is difficult to simulate at present[15]. Third, the thermal conductivity is obtained by constructing typical structural units corresponding to the aerogel microstructure. We simplify the complex nano porous structure of aerogel material into a regular unit model, and then obtain the combined thermal conductivity of gas phase and solid phase by using the equivalent resistance method based on the known structural parameters. For example, Zeng used three types of cubic arrays of intersecting square bars, intersecting column bars, and intersecting spheres to characterize the structure of silica aerogel[16]. Wei used the intersecting spheres proposed by Zeng[16] cubic arrays to analyze the structural models of silica aerogels, hard calcium silicate, and hard calcium silicate aerogels, and then the equivalent resistance method to obtain the analytical expressions for their effective thermal conductivity[17]. Dan proposed a new effective model, the spherical hollow cube model, based on the structure of aerogels, and used the equivalent circuit method to deduce the thermal conductivity of different types of aerogels[18]. The microstructure is used to calculate the thermal conductivity of aerogel, with the advantages of high accuracy, economic effectiveness, controllability, and scalability. However, for aerogel materials with different microstructures, the structural parameters and the impact of thermal properties (gas phase and solid phase thermal conductivity) on the total thermal conductivity of materials should be determined, and different basic structural models should be built.
Fractal geometry theory is a mathematical tool used to describe the repeatability of self-similarity structures at different scales. Remarkably, compared with the method of constructing typical structural units corresponding to the microstructure of aerogel, the fractal geometry theory can calculate the thermal conductivity of porous materials without accurately obtaining the structural parameters of porous materials. The fractal geometry theory is a self-similarity model, which aims to use the iterative method to simulate the internal pore structure of porous materials and establish the effective thermal conductivity of porous medium, with less errors between the model prediction results and the experimental data. For instance, Pia proposed a primitive mixed fractal model to predict the thermal conductivity of porous ceramic materials, which can serve as a microstructure simulator to improve the thermal performance of porous ceramic materials [19]. Feng and Ma established a self-similarity model for the effective thermal conductivity of porous medium based on the thermoelectric analogy technology and self-similarity of the Sierpinski carpet, whose prediction agreement well with the experimental data [20, 21]. Qin established two types of fractal models, namely, parallel and serial, which intend to predict the effective thermal conductivity of a new type of aerogel sample data into the proposed thermal conductivity prediction model and compare the error of the model with that of other scholars’ thermal conductivity prediction models. Therefore, the fractal unit structure of aerogel is superior than the thermal conductivity prediction model of 3 × 3. The research results indicate that the k × k Sierpinski carpet model is a creative method to improve the accuracy of the model for predicting the thermal conductivity of aerogel materials and provides more computational model ideas for investigating more thermal conductivity of other porous materials.

2. Establishment of Thermal Conductivity Prediction Model

2.1. Fractal process of Sierpinski carpet with fractal unit structure of k × k

To find the fractal unit structure suitable for porous medium materials with high porosity, the most fundamental 3 × 3 Sierpinski carpet is used as an extension, and the k × k Sierpinski carpet composed of fractal units is adopted to characterize porous medium materials. The Sierpinski carpet model (denoted as SC) is obtained by repeatedly removing the square from the initial stage with a unit side length, whose iterative generation description is shown in Figure 1. (a) is a square with a side length of L, and a rectangle with a side length of C is removed from its center, where C = 1 and L = 3. The black area includes the remaining eight sub squares with unit side length C. The first iteration is completed by removing the 8C² sub squares from their center sub squares and using the initial method to obtain some smaller sub squares with unit side length. During the second iteration, we continue to remove the centers of these smaller sub squares with unit side lengths, and the iterative process can be executed toward infinity.

![Figure 1. Sierpinski carpet model](image)

This study only considers Sierpinski carpets composed of odd fractal units due to the diversity of Sierpinski carpets composed of even fractal units. When k > 1 is a positive integer and an odd number, initially, the Sierpinski carpet composed of k × k fractal units is a square with a side length of 1. In the first iteration, the center of the square with a side length of 1 is removed, and the remaining 8C² sub squares are used as the initial method to find the fractal unit structure suitable for porous medium materials with high porosity. The optimal fractal unit was optimized by the minimum difference error between the porosity after Sierpinski carpet iteration and the actual porosity, thereby selecting the appropriate fractal structure to obtain its thermal conductivity. In the application and verification of thermal conductivity prediction model, we substitute four types of aerogel sample data into the proposed thermal conductivity prediction model and compare the error of the model with that of other scholars’ thermal conductivity prediction models. Therefore, the fractal unit structure k × k is superior than the thermal conductivity prediction model of 3 × 3. The research results indicate that the k × k Sierpinski carpet model is a creative method to improve the accuracy of the model for predicting the thermal conductivity of aerogel materials and provides more computational model ideas for investigating more thermal conductivity of other porous materials.
length of 1 is removed by a square with a side length of $1/k$. In the second iteration, according to the former method in the first iteration, we remove the remaining $k^2 - 1$ squares with side lengths of $1/k$ by subtracting their center side lengths of $(1/k)^2$. Therefore, the Sierpinski carpet fractal unit with a fractal unit structure for a $k \times k$ is shown in Figure 2, where the black area represents the area of the solid phase (porous material skeleton), which is the removed part. The blank area represents the gas phase (pore) area, which is a square with a starting edge length of 1.

![Figure 2. Sierpinski carpet with fractal unit of $k \times k$.](image)

2.2. Establishment of thermal conductivity model based on equivalent resistance method

The equivalent resistance diagrams were obtained using the equivalent resistance method to establish the thermal resistance network model of the basic fractal units on the surface and inside the aerogel. On the basis of the $k \times k$ fractal unit structure Sierpinski Carpet on the first step, its equivalent resistance diagram can be drawn as follows Figure 3:

![Figure 3. Fractal unit structure of a first-order $k \times k$ and equivalent resistance diagram of the first order Sierpinski Carpet](image)

According to the $k \times k$ fractal unit structure of Sierpinski carpet and equivalent resistance diagram in order 1, we assume that $\bar{c}$ is conductivity, and $\bar{R}$ is the average resistance[18]. According to the calculation formula of parallel resistance, the following can be concluded:

$$\bar{c} = \frac{1}{\bar{R}} = \frac{1}{R_1} + \frac{1}{R_2} + \cdots + \frac{1}{R_k}$$  \hspace{1cm} (1)

According to the formula for calculating series resistances, the following can be inferred:

$$\begin{cases} R_1 = R_2 = \cdots = R_{k+1} = R_{k+3} = \cdots = R_k = R_k + R_k + \cdots + R_k = k \cdot R_k \\ R_{k+1} = R_k + R_k + \cdots + R_k + R_k + \cdots + R_k = (k - 1) \cdot R_k + R_k \end{cases}$$  \hspace{1cm} (2)

By combining formulas (1) and (2), the following can be reached obtained:

$$\bar{c} = \frac{k - 1}{k \cdot R_k} + \frac{1}{(k - 1) \cdot R_k + R_k}$$  \hspace{1cm} (3)

According to the equivalent resistance method, as follows:

$$\bar{R} = R_{eff} \cdot \frac{l}{\alpha}$$  \hspace{1cm} (4)

where $R_{eff}$ is the "total" resistance, $R_f$ is the gas resistance, $R_s$ is the solid resistance, $l$ is the length of porous medium material, and $\alpha$ is the cross-sectional area in general. By substituting formula (4) into formula (3) and assuming that each unit resistance is the same, we can obtain:

$$\frac{1}{R_{eff} \cdot \frac{l}{\alpha}} = \frac{k - 1}{k \cdot R_f \cdot \frac{l}{\alpha}} + \frac{1}{(k - 1) \cdot R_f \cdot \frac{l}{\alpha} + R_s \cdot \frac{l}{\alpha}}$$  \hspace{1cm} (5)

namely,
\[
\frac{1}{R_{\text{eff}}} = \frac{k_1 - 1}{k_2 \cdot R_f} + \frac{1}{(k_1 - 1) \cdot R_f + R_s}
\]

(6)

The relationship between thermal conductivity and resistance indicates the following:

\[
k_{\text{eff}} = \frac{1}{R_{\text{eff}}}
\]

(7)

Substituting formula (7) into formula (6) yields the following:

\[
\frac{1}{k_{\text{eff}}} = \frac{k - 1}{k \cdot k_f} + \frac{1}{(k - 1) \cdot k_f + \frac{1}{k_s}}
\]

(8)

The thermal conductivity model of the first-order Sierpinski carpet based on the equivalent resistance method can be derived as follows:

\[
k_{\text{eff}} = \frac{k - 1}{k} \cdot k_f + \frac{k_s \cdot k_f}{(k - 1) \cdot k_s + k_f}
\]

(9)

where \(k_{\text{eff}}\) represents the thermal conductivity of the first-order \(k \times k\) Sierpinski carpet calculated based on the equivalent resistance method, \(k_f\) represents the solid phase thermal conductivity, and \(k_s\) represents the gas phase thermal conductivity.

To achieve an overall porosity abysmally that is close to the actual porosity of porous medium materials \(\phi\), we iterated the basic fractal unit of the Sierpinski carpet periodically. It should be noted that the aerogel materials in this paper are all of high porosity structure, so the influence of solid part on overall thermal conductivity can be properly ignored. After the iteration, the first basic fractal unit is not only a part of the next stage of fractal modeling, but also of “gas.” Therefore, \(k_f\) is equal to the previously calculated \(k_{\text{eff}}\). The value of \(k_{\text{eff}}\) calculated in the \(n\)th iteration will be inserted into step \((n + 1)\) by using the same simple expression, serving as the new value for the “gas phase” conductivity[24-26], as follows:

\[
k_{\text{eff}}(n) = k_f(n + 1)
\]

(10)

Then, the heat conduction model of the porous medium is based on the equivalent resistance method, and the \(k \times k\) Sierpinski carpet with fractal unit structure is as follows:

\[
k_{\text{eff}}(n) = k_f(n + 1) = \frac{k - 1}{k} \cdot k_f(n) + \frac{k_s \cdot k_f(n)}{k \cdot k_s + k_f(n)}
\]

(11)

where \(k_{\text{eff}}(n)\) represents the thermal conductivity of the porous medium predicted by the \(k \times k\) Sierpinski carpet with fractal unit structure in the \(n\)th iteration, \(k_f(n + 1)\) represents the gas thermal conductivity calculated by the \(n + 1\)th iteration, and \(k_s\) represents the solid thermal conductivity.

2.3. Optimization of the best fractal unit structure

Sierpinski carpet is an internal microscopic material used to characterize porous medium materials; it is constructed from porosity. When a more precise porosity of Sierpinski carpet approaches the porosity of porous medium materials, perfect characterization effect is shown. Therefore, we use the difference between the porosity after the Sierpinski carpet iteration and the actual porosity to optimize the optimal fractal unit. When the difference is small, the internal structure of the porous medium materials is effectively characterized. Hence, the thermal conductivity calculated by the model is accurate. The appropriate fractal structure can be selected in light of the porosity of porous medium materials to achieve its thermal conductivity.

Assuming that the actual porosity of a porous medium material is \(\phi_0\), in the \(k \times k\) Sierpinski carpet with iteration number of 1, the proportion of solid phase is \(1/k^2\). Thus, the pore proportion is as follows:

\[
\phi_1 = 1 \cdot \frac{k^2 - 1}{k^2} = \frac{k^2 - 1}{k^2}
\]

(12)

After \(n\) iterations, the porosity of Sierpinski carpet is as follows:

\[
\phi_n = \left(\frac{k^2 - 1}{k^2}\right)^n
\]

(13)

Suppose that the gap between the actual porosity of the sample and the porosity after Sierpinski carpet iteration is \(t\), as the following can be derived:

\[
t = \phi_0 - \phi_n = \phi_0 - \left(\frac{k^2 - 1}{k^2}\right)^n
\]

(14)

where \(k > 1\) is a positive integer and an odd number, \(n\) is a positive integer, \(\phi_0\) is the actual porosity of the sample, and \(\phi_n\) is the porosity after the \(n\)th iteration of \(k \times k\) Sierpinski carpet.

According to the relationship between the difference in porosity and thermal conductivity in the three-box model [24], we can obtain the dimension (\(k\)) and iteration number (\(n\)) of the optimal fractal unit structure.

\[
\min t = \phi_0 - \left(\frac{k^2 - 1}{k^2}\right)^n
\]

(15)

s.t.

\[
\begin{cases}
  k > 1 & \text{is a positive integer and is odd,} \\
  n \geq 1 & \text{is a positive integer,} \\
  \phi_0 > \left(\frac{k^2 - 1}{k^2}\right)^n.
\end{cases}
\]

(16)

The optimization model is applied to obtain \(k\) and \(n\), which are used to calculate the thermal conductivity.

3. Application and Validation of the Thermal Conductivity Prediction Model

The established thermal conductivity prediction model to four reported aerogel materials, including aramid nanofiber aerogel (ANFAs)[24], hydrophobic cellulose silica composite aerogel (BC-FS)[27], polyimide aerogel (IBNR-PI)[30], and C/SiC Aerogel[31], is used to verify the applicability of the proposed model. The solid phase thermal conductivity, porosity, and actual thermal conductivity of each aerogel are demonstrated in Table 1.
Table 1. Sample data [24,38-34]

<table>
<thead>
<tr>
<th>sample name</th>
<th>Solid phase thermal conductivity (Wm(^{-1})K(^{-1}))</th>
<th>porosity</th>
<th>Real thermal conductivity (Wm(^{-1})K(^{-1}))</th>
</tr>
</thead>
<tbody>
<tr>
<td>ANFAs</td>
<td>2.064191</td>
<td>0.9931</td>
<td>0.02935</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.990752</td>
<td>0.031334</td>
</tr>
<tr>
<td>BC-FS</td>
<td>15</td>
<td>0.9819</td>
<td>0.032</td>
</tr>
<tr>
<td>IBNR-PI</td>
<td>0.44</td>
<td>0.9492</td>
<td>0.03006</td>
</tr>
<tr>
<td>Cf/SiC</td>
<td>3.95</td>
<td>0.995</td>
<td>0.033</td>
</tr>
</tbody>
</table>

Based on the porosity and solid-phase thermal conductivity data of the 8 samples in Table 1, the optimal fractal unit structure and iteration number of the 8 samples were calculated through formulas (15) and (16). The results are demonstrated in Table 2.

Table 2. Average tortuosity calculation results of 14 samples

<table>
<thead>
<tr>
<th>sample name</th>
<th>porosity</th>
<th>Optimal Fractal Unit Structure</th>
<th>iterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>ANFAs</td>
<td>0.9931</td>
<td>17x17</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>0.990752</td>
<td>17x17</td>
<td>3</td>
</tr>
<tr>
<td>BC-FS</td>
<td>0.9819</td>
<td>19x19</td>
<td>7</td>
</tr>
<tr>
<td>IBNR-PI</td>
<td>0.9492</td>
<td>21x21</td>
<td>23</td>
</tr>
<tr>
<td>Cf/SiC</td>
<td>0.995</td>
<td>19x19</td>
<td>2</td>
</tr>
</tbody>
</table>

To determine whether the change in fractal unit structure can effectively predict the thermal conductivity of aerogel, we compared the thermal conductivity prediction model of Chen Xiao [24] in the previous work. The finding shows that when the fractal unit structure is 3 x 3, the error between the
predicted thermal conductivity of the optimal aerogel and the actual thermal conductivity is as illustrated in Table 4.

<table>
<thead>
<tr>
<th>sample name</th>
<th>porosity</th>
<th>$k_{\text{real}}$ ($W m^{-1} K^{-1}$)</th>
<th>$k_{\text{effd}}$ ($W m^{-1} K^{-1}$)</th>
<th>$\epsilon (3 \times 3)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>ANFAs</td>
<td>0.9931</td>
<td>0.02935</td>
<td>0.0287</td>
<td>0.0209</td>
</tr>
<tr>
<td></td>
<td>0.990752</td>
<td>0.03134</td>
<td>0.0295</td>
<td>0.059</td>
</tr>
<tr>
<td></td>
<td>ANFAs</td>
<td>0.99057</td>
<td>0.03202</td>
<td>0.0295</td>
</tr>
<tr>
<td></td>
<td>0.990509</td>
<td>0.033046</td>
<td>0.0295</td>
<td>0.0799</td>
</tr>
<tr>
<td></td>
<td>0.989372</td>
<td>0.033513</td>
<td>0.0295</td>
<td>0.0932</td>
</tr>
<tr>
<td>BC-FS</td>
<td>0.9819</td>
<td>0.032</td>
<td>0.05774</td>
<td>0.3042</td>
</tr>
<tr>
<td>IBNR-PI</td>
<td>0.9492</td>
<td>0.03006</td>
<td>0.03354</td>
<td>0.1156</td>
</tr>
<tr>
<td>CF/SiC</td>
<td>0.995</td>
<td>0.033</td>
<td>0.0285</td>
<td>0.1363</td>
</tr>
</tbody>
</table>

a) Real thermal conductivity
b) Predicted thermal conductivity of the model with a fractal unit structure of $3 \times 3$;
c) Error rate of the thermal conductivity model with $3 \times 3$ fractal unit structure

Table IV shows the error relationship between experimental data and the aerogel thermal conductivity model of Sierpinski carpet based on fractal units of $3 \times 3$, whose relative error is controlled between 2.09% and 80.42%, and the average relative error is 17.35%. Therefore, the analysis of four different aerogels indicates that the average relative error of this prediction model decreased by 11.58% compared with the fractal geometry thermal conductivity prediction model of $3 \times 3$. Especially for the hydrophobic cellulose silica composite aerogel (BC-FS) with a porosity of 98.19%, the error between the calculated results and the actual thermal conductivity using the previous thermal conductivity model of the Sierpinski carpet with a fractal cell structure of $3 \times 3$ is as high as 80.42%. However, the error is only 5.59% under the improved model in this paper, whose rate is reduced by 74.83%, showing a significant effect. The specific results are demonstrated in the following figure 4:

![Figure 4. Error comparison of different model results with experimental data](image)

4. Conclusions

A prediction model of thermal conductivity of aerogel is established based on Sierpinski carpet with fractal unit structure of $k \times k$ and equivalent circuit method. Then, the optimal fractal unit structure of aerogel carpet is calculated through the aerogel porosity. Finally, on the basis of the sample data of four different aerogels, the relative error of the proposed thermal conductivity prediction model established was found to be 1.58%-9.78%, and the average error of the thermal conductivity prediction model is 5.77%, moreover, its average error is 11.58% lower than that of thermal conductivity prediction model established by Sierpinski carpet with $3 \times 3$ cell structure. This finding embodies that the proposed thermal conductivity prediction model of aerogel established is effective and reliable.

Results show that the fractal structure of Sierpinski pet has a certain influence on the prediction of thermal conductivity of aerogel, and provides more computational model ideas for the study of thermal conductivity of other porous materials. Through the establishment of pore fractal model and calculation simulation, we can predict the thermal conductivity of aerogel materials with different pore sizes and study the change trend of thermal conductivity with the change in pore size distribution.

Acknowledgment

The authors would like to thank the National Natural Science Foundation of China (52273059) and the Science and Technology Plans of Tianjin (23JCYBJC01030) for their financial supports.

Conflict of interest

The authors have no conflicts to disclose.

Data availability

The data that supports the findings of this study are available within the article.

References


