NUMERICAL STUDY ON EFFECTIVE THERMAL CONDUCTIVITY OF THREE-DIMENSIONAL FINE-KNITTED PERFORATED C/SIC COMPOSITE MATERIALS

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C/SiC composite materials have the advantages of high temperature resistance, low expansion, and excellent thermal stability, and are widely used in aerospace, military, energy and other fields. The thermal conductivity of C/SiC composite materials is an important characteristic to ensure the stable operation of thermal protection structures in high-temperature environments. In order to investigate the effects of carbon fiber volume fraction and yarn porosity on the effective thermal conductivity of composite materials, a three-dimensional fine-knitted perforated C/SiC (3DP C/SiC) composite materials cell model was established. The in-plane and out of plane thermal conductivity of the composite materials were calculated. The results indicate that the out of plane thermal conductivity is smaller than the in plane thermal conductivity. The difference between in-plane thermal conductivity and out of plane thermal conductivity decreases as the external porosity of the yarn increases. Additionally, the influence of carbon fiber volume fraction and yarn porosity on the effective thermal conductivity of composite materials was numerically studied. The results indicate that as the volume fraction of carbon fiber and the porosity inside and outside the yarn increase, the in-plane and out of plane thermal conductivity of the composite materials both decrease. In addition, the effective thermal conductivity of 3DP C/SiC composite considering the pores in the yarn is lower than that without considering the pores in the yarn.
Key words: *numerical research*, *unit cell model, effective thermal conductivity*, *three-dimensional fine-knitted perforated composite materials*

1. Introduction

As a typical continuous fiber reinforced ceramic matrix composite materials, carbon fiber reinforced SiC (C/SiC) composite materials have many excellent physical properties, such as low density, high toughness, high thermal stability, low coefficient of expansion, high corrosion resistance, thermal shock resistance, and delamination resistance [1-3]. Therefore, C/SiC composite materials are gradually becoming the preferred material for thermal protection components, applied in fields such as aviation engines [4], thermal protection structures [5,6], hypersonic aircraft [7], and so on. According to the different types of fiber weaving, C/SiC materials can be divided into 2D plain weave C/SiC, 2.5D C/SiC, and 3D C/SiC. Compared with 2D braided C/SiC composite, 2.5D and 3D C/SiC composite exhibit excellent delamination resistance and interlayer shear stress [8,9]. As a representative of three-dimensional fabric reinforced ceramic matrix composite, three-dimensional fine-knitted perforated C/SiC (3DP C/SiC) composite have shown unique advantages. When composite materials are used as thermal resistance materials, their thermal conductivity is of great significance for the thermal performance/safety design of aircraft. In order to optimize the structure of composite materials, it is necessary to compare and study the thermal conductivity of C/SiC composite materials with different prefabricated structures.

Although experimental testing can effectively explore the macroscopic properties of materials [10-12], it requires significant time and funding investments, while only a limited number of material types can be studied, making it difficult to establish quantitative relationships between material systems and properties. Therefore, in the past decade or so, many microscale and mesoscale analysis methods have been applied to calculate the thermal conductivity of composite materials. Microscale analysis methods have been utilized by Sun et al. [13] to establish a series of theoretical models for exploring the thermal conductivity of unidirectional composite materials. However, existing theoretical methods are constrained by the complex structures of composite materials, preventing accurate calculations of thermal conductivity for those with more intricate configurations. In order to solve this, numerical analysis methods have been adopted by some researchers to explore the properties of composite materials [14,15]. Based on multiscale numerical methods, a thermomechanical multiscale model is developed by Penide-Fernandez et al. [16] to predict the out-of-plane thermal conductivity at the micro and meso-levels of transversely loaded two-dimensional woven ceramic fabrics. A three-dimensional finite volume numerical model is proposed by Liu et al. [17] through the reconstruction of porosity inside and outside the yarn, and the upscale method is utilized to predict the thermal conductivity of SiC matrix, woven yarn, and plain C/SiC composite materials. The thermal conductivity of three-dimensional four-way braided composite materials is investigated by Gou et al. [18] using the finite element method. In addition, A micromechanical model is proposed by Xu et al. [19] that considers PyC interphase thermal conductance and manufacturing-induced voids to predict the thermal conductivity of C/SiC composite. The thermal conductivity of 2.5D AWC along the warp, weft, and thickness directions is investigated by Dong et al. [20] through experiments and finite element analysis. The effect of graphite crystal development on the thermal response behavior of controllable graphitized HTC-C/C composite is examined by Wang et al. [21], who find that the out-of-plane thermal conductivity is primarily influenced by porosity. Additionally, Zhou et al. [22] determine that pore morphology has minimal effect on the effective thermal conductivity. These studies have demonstrated that thermal conductivity is greatly influenced by fiber volume fraction and porosity, with an increase in porosity and a decrease in thermal conductivity. The pore shape has almost no effect on these key influencing factors. Furthermore, these studies inspire the establishment of an accurate geometric model of pores [19] or an equivalent pore matrix model [14,17]. These methods can be employed to create an equivalent model that incorporates both the matrix and pores to investigate the effect of porosity on thermal conductivity.

However, the influence of internal pores in fine-knitted perforated C/SiC composite materials on the effective thermal conductivity of in-plane and out-of-plane anisotropic composite materials has not been considered by most researchers, and there is relatively little research on the effects of porosity and fiber volume fraction on the thermal conductivity of 3DP composite materials. In this work, the unit cell model was established to predict the effective thermal conductivity of 3DP C/SiC composite materials. The thermal conductivity of the composite materials was numerically calculated using finite volume method. In addition, the effects of carbon fiber volume fraction, yarn internal and external pores on the in-plane and out of plane thermal conductivity of 3DP C/SiC composite were studied. This method can provide guidance for the thermal analysis and design of 3DP composite materials in engineering.

2. Physical problem description and numerical model

2.1. Geometric model of woven C/SiC composite materials

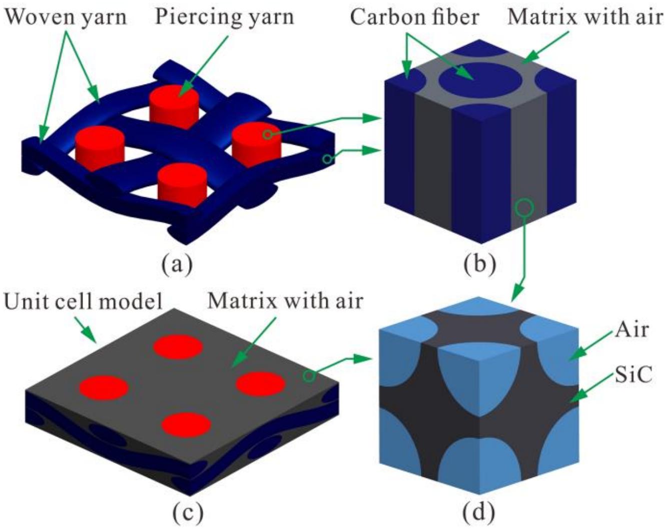

Figure 1. Structure and composition of 3DP C/SiC composite materials (a) Yarn of 3DP composite materials, (b) Unit cell model of yarn, (c) Unit model of 3DP composite materials, (d) Unit model of matrix

The geometric structure of 3DP composite materials is complex, and thermal conductivity exhibits anisotropy. A multi-scale model of composite materials is established in this article, and finite element methods are used to study and analyze the performance of composite materials. The structure and composition of 3DP C/SiC composite materials are shown in Fig. 1, which consisting of interwoven woven yarn, perforated yarn, and SiC matrix. Woven yarn and perforated yarn are composed of carbon fiber and SiC matrix, interwoven woven yarn is stacked together and sewn by perforated yarn that runs through the thickness. In the manufacturing process of composite materials, some pores occupied by air will form in the matrix [23]. When numerically solving the thermal conductivity of 3DP C/SiC composite materials, the influence of small amounts of free silicon and carbon is ignored.

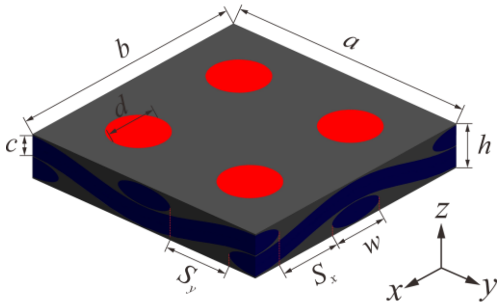

Figure 2. Unit cell model of 3DP C/SiC composite materials

In order to calculate the effective thermal conductivity of 3DP C/SiC composite materials, it is necessary to first establish a unit cell model of SiC matrix (Fig. 1 (d)) and a unit cell model of yarn (Fig. 1 (b)). In Fig. 1 (b), the unit cell model of the yarn is composed of carbon fibers and SiC matrix, which also contains a small amount of air [24]. For the unit cell model, the central cylinder and four 1/4 cylinders are made of carbon fiber, while the rest are made of SiC matrix. Assuming the fiber volume fraction of 3DP composite materials φ_f is 0.3-0.38. In Fig. 1 (d), it is assumed that air is uniformly distributed in the SiC matrix, with eight 1/8 spheres representing air and the rest being SiC. The SiC matrix exists on the outside of the yarn as well as in the woven and puncture yarns. Assuming that the porosity inside and outside the yarn is 0-0.01 and 0-0.25, respectively.

A unit cell model of 3DP C/SiC composite materials is established. The in-plane and out of plane thermal conductivity of the composite materials are calculated. Figure 2 shows the unit cell model of 3DP composite materials based on measured values [25]. a and b are lengths of the unit cell model, and h is the height of the unit cell. c and w are the height and width of the woven yarn, respectively. S_x and S_y are distances between two adjacent yarns in x and y directions, respectively. d is the diameter of the perforated yarn. The values of geometric parameters are shown in Table 1. The range of variation of woven yarn in the z-direction is defined by Eq. (1). The cross-section of the yarn is defined as $-w/2 < x < w/2$ and $-w/2 < y < w/2$.

$$z = \pm\frac{c}{2}\cos\left(\pi x / 2a\right),\ z = \pm\frac{c}{2}\cos\left(\pi x / 2b\right) \tag{1}$$

Table 1. Geometric parameters of unit cell model

Parameter	a	b	h	c	w	S_x	S_y	d
Value (mm)	2.60	2.60	0.44	0.20	0.61	0.69	0.69	0.58

2.2. Numerical calculation of effective thermal conductivity

The 3DP C/SiC composite materials are composed of carbon fiber and SiC matrix mixed with air. The thermal conductivity of these three substances at 300K is shown in Table 2 [26]. Before calculating the effective thermal conductivity of 3DP C/SiC composite materials, it is necessary to first calculate the thermal conductivity of the matrix and yarn.

Table 2. Thermal conductivities of carbon fiber, SiC and air

Materials	Diameter, μm	Transverse thermal conductivity, [$Wm^{-1}K^{-1}$]	Axial thermal conductivity, [$Wm^{-1}K^{-1}$]
Carbon fiber	6.9	0.675	7.81
SiC	/	70	70
Air	/	0.024	0.024

2.2.1 Thermal conductivity of SiC matrix

As shown in Fig. 3, a cell model of SiC matrix is established to calculate the effective thermal conductivity of the matrix. In this cubic model, it is assumed that the spherical pores are uniformly distributed and the dimensionless length of the unit cell is 1. To calculate the thermal conductivity of matrices with different porosity, the pore sizes r_1 and r_2 of the internal and external unit cells of the yarn were calculated using Eq. (2) and Eq. (3), respectively.

$$\frac{\varphi_i}{\varphi_y} = \frac{4\pi r_1^3 / 3}{1} \tag{2}$$

$$\frac{\varphi_o}{1-\varphi_y} = \frac{4\pi r_2^3 / 3}{1} \tag{3}$$

Among φ_i andφ_o is the porosity inside and outside the yarn, respectively. r_1 and r_2 are the pore

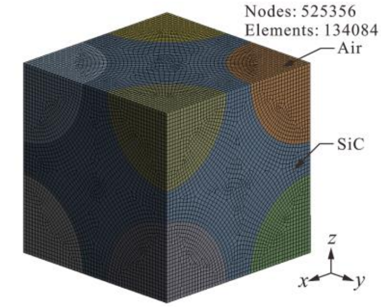

Figure 3. Mesh of the unit cell model of the SiC matrix

sizes of the unit cells of the matrix inside and outside the yarn, respectively. φ_y is the yarn volume fraction of 3DP C/SiC composite materials, is calculated based on the geometric parameters of 3DP C/SiC composite materials. Taking a porosity of 0.15 as an example, the unit cell model grid of the matrix is shown in Fig. 3. Independence of the matrix grid is verified by applying temperature boundary conditions on the model surface in the z-axis direction and adiabatic boundary conditions on the remaining surfaces of the model. According to the Fourier thermal conductivity law expressed in Eq. (4), obtain temperature gradient ∇T and corresponding heat flux q to determine effective thermal conductivity of the SiC matrix.

$$\boldsymbol{q} = -\lambda \nabla T \tag{4}$$

2.2.2 Thermal conductivity of yarn

As shown in Fig. 4, cell models were established for both woven and perforated yarns to predict their axial and transverse thermal conductivity. The yarn is composed of carbon fiber and silicon carbide matrix, and the thermal conductivity of carbon fiber and SiC matrix is the input parameter for calculating the effective thermal conductivity of the yarn. Taking carbon fiber volume fraction of 0.3 as an example, the unit cell model mesh of the yarn is shown in Fig. 4. And verified the independence of the yarn mesh. To obtain axial thermal conductivity λ_a. The temperature boundary conditions are applied along the z-axis to the surface of the yarn element model, while the adiabatic boundary conditions are applied to the remaining surfaces of the element model. In order to obtain lateral thermal conductivity λ_t. Temperature boundary conditions are applied along the x-axis (or y-axis) to the surface of the element model, while adiabatic boundary conditions are applied to the remaining surfaces of the element model. The effective thermal conductivity of woven and perforated yarns is calculated using the Fourier heat conduction law represented in Eq. (4).

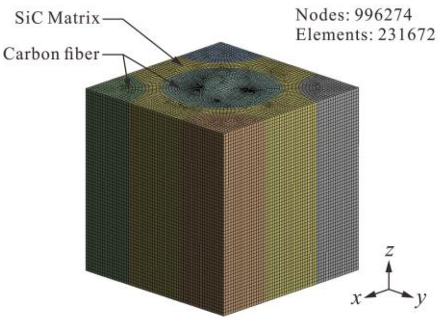

Figure 4. Mesh of yarn unit model

2.2.3 Thermal conductivity of 3DP C/SiC composite materials

A cell model for 3DP composite materials are established to predict their in-plane and out of plane thermal conductivity. Composite materials are composed of interwoven woven yarns, perforated yarns, and SiC matrix outside the yarns. The effective thermal conductivity of woven yarn, perforated yarn, and SiC matrix is an input parameter for calculating the effective thermal conductivity of 3DP composite materials. The mesh of the composite materials unit model is shown

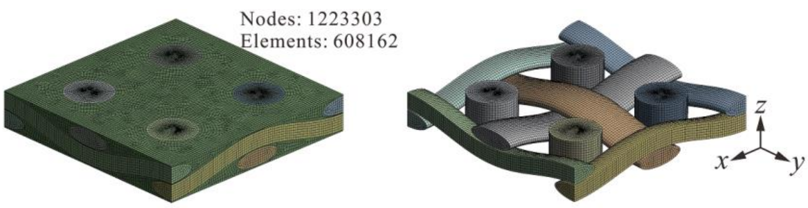

Figure 5. Grid of unit cell for 3DP C/SiC composite materials

in Fig. 5. Steady state thermal analysis of 3DP composite materials is conducted using Fluent software. The conduction control equation is Eq. (5). Where T is the temperature, λ_{xx}, λ_{yy}, λ_{zz}, are the anisotropic thermal conductivity of composite materials. To obtain out of plane thermal conductivity λ_{zz}, temperature boundary conditions are applied along the z-axis to the surface of the model, while adiabatic boundary conditions are applied to the remaining surfaces of the model [27]. To obtain in-plane thermal conductivity λ_{xx} and λ_{yy}, it is necessary to apply temperature boundary conditions along the x-axis (or y-axis) on the surface, and specify adiabatic boundary conditions on the remaining surfaces of the model. Effective thermal conductivity of composite materials λ_{xx}, λ_{yy} and λ_{zz} is obtained based on the Fourier heat conduction law shown in Eq. (4).

$$\lambda_{xx}\frac{\partial^2 T}{\partial x^2}+\lambda_{yy}\frac{\partial^2 T}{\partial y^2}+\lambda_{zz}\frac{\partial^2 T}{\partial z^2}+\left(\lambda_{xy}+\lambda_{yx}\right)\frac{\partial^2 T}{\partial x\partial y}+\left(\lambda_{xz}+\lambda_{zx}\right)\frac{\partial^2 T}{\partial x\partial z}+\left(\lambda_{yz}+\lambda_{zy}\right)\frac{\partial^2 T}{\partial y\partial z}=0 \quad (5)$$

2.2.4. Prediction model validation

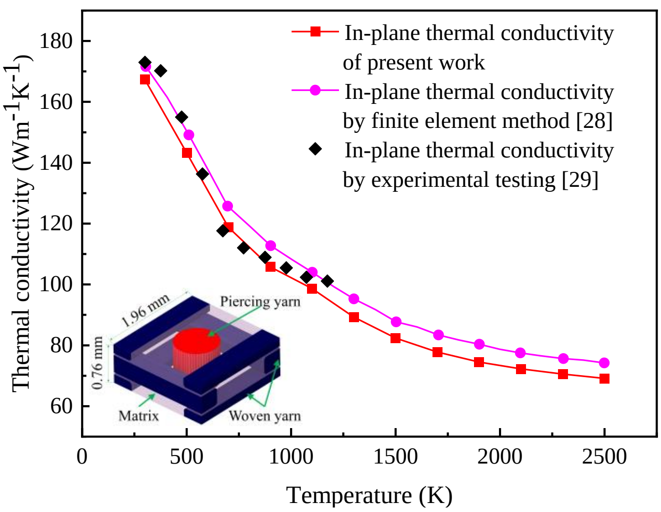

Figure 6. Thermal conductivities between the prediction model and the reference

This study employs the finite volume method, using Fluent software and the SIMPLE algorithm to calculate the thermal conductivity. In order to verify the accuracy and validity of the numerical method, void/matrix models are reconstructed based on the dimensions and material properties from Ai et al. [28] and Luo et al. [29]. The thermal conductivity obtained using the numerical method described in this study is compared with the finite element simulation results [28] and experimental testing [29] from the literature. The comparison between simulation and experimental results is detailed in Figure 6, which confirms the correctness of the calculated thermal conductivity.

3. Results and discussion

In this work, the porosity inside and outside the yarn is assumed to range from 0 to 0.01 and 0 to 0.25, respectively, for the 3DP C/SiC composite. The carbon fiber volume fraction is assumed to range from 0.3 to 0.38. The comparison between the in-plane thermal conductivity and the out-of-plane thermal conductivity is investigated. The effects of porosity and carbon fiber volume fraction on the effective thermal conductivity of the 3DP C/SiC composite are also researched in the following sections.

3.1. Comparison between the in-plane and out-of-plane thermal conductivity

Figure 7 makes a contrastive analysis of the in-plane and the out-of-plane thermal conductivity about the effect of the porosity inside and outside the yarn on the effective thermal conductivity for the 3DP C/SiC composite. As shown in Fig. 7, the in-plane and out-of-plane thermal conductivity of the composite both decrease with the increase of the porosity outside the yarn. The thermal conductivity when considering the pores inside the yarn is smaller than that when not considering pores inside the yarn. The reason is that the thermal conductivity of air is smaller than the thermal conductivity of the SiC. The effective thermal conductivity of the SiC matrix decreases as the porosity increases. Consequently, the effective thermal conductivity of the C/SiC composite decreases with the decrease of the thermal conductivity of the SiC matrix. In addition, the in-plane thermal conductivity (λ_{xx}, λ_{yy}) is larger than the out-of-plane thermal conductivity (λ_{zz}) for the 3DP C/SiC composite. And this result is also observed in the plain woven C/SiC composite [26]. This can be explained that the axial direction of the carbon fiber mostly distributes along the in-plane direction and the axial thermal conductivity is much larger than the transverse thermal conductivity for the carbon fiber. From Fig. 7, it is also concluded that the difference between the in-plane thermal conductivity and out-of-plane thermal conductivity decreases with the increase of the porosity φ_o. The reason for this variation tendency is that the porosity gradually becomes the dominant factor to determinate the thermal conductivity with the increase of porosity.

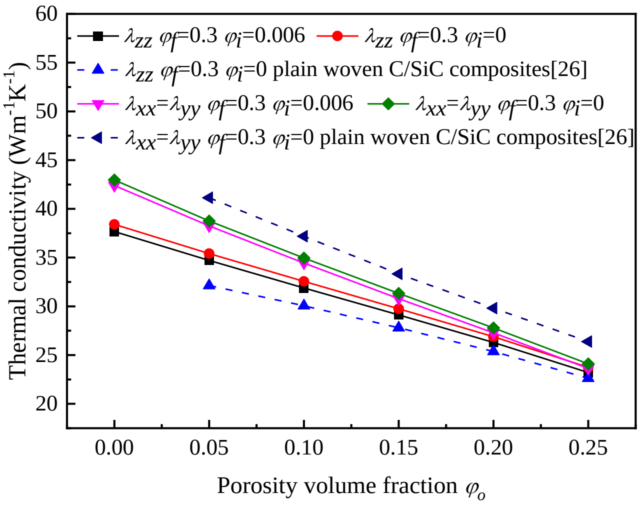

Figure 7. Comparison of in-plane and out-of-plane conductivity for the C/SiC composite

3.2. Effect of the porosity inside the yarn on the thermal conductivity

Figure 8 illustrates the relationship between the out-of-plane thermal conductivity λ_{zz} and the inside porosity φ_i with various carbon fiber volume fraction φ_f. The outside porosity φ_o is equal to 0.15. As shown in Fig. 8, the out-of-plane thermal conductivity of the composite decreases with the increase of the porosity φ_i. For the different carbon fiber volume fraction 0.3, 0.32, 0.34, 0.36, and 0.38, the out-of-plane thermal conductivity decreases by 3.4%, 3.7%, 3.9%, 4.1% and 4.0% when the porosity φ_i increase from 0 to 0.01. This can be explained that the thermal conductivity of the air is smaller than that of the SiC. Thus, the thermal conductivity of the SiC matrix decreases with the increase of the porosity φ_i. Thus, the thermal conductivity of SiC matrix decreasing results in the decrease of out-of-plane thermal conductivity. In addition, the out-of-plane thermal conductivity of the composite decreases with the increase of the

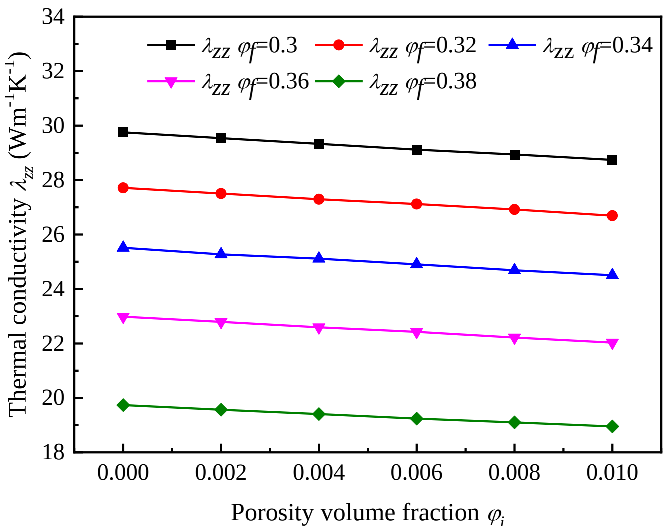

Figure 8. Relationship between out-of-plane thermal conductivity λ_{zz} and porosity inside the yarn φ_i with different carbon fiber volume fraction φ_f

carbon fiber volume fraction. The reason for this result is that the thermal conductivity of the carbon fiber is smaller than that of the SiC matrix. And the thermal conductivity of the yarn decreases with the increase of the carbon fiber volume fraction. The decrease of the thermal conductivity of the yarn causes the decrease of the out-of-plane thermal conductivity.

Figure 9 shows the relationship between the in-plane thermal conductivity (λ_{xx}, λ_{yy}) and the porosity inside the yarn φ_i with different carbon fiber volume fraction φ_f. The porosity outside the yarn φ_o is equal to 0.15. The in-plane thermal conductivity decreases with the increase of the porosity φ_i. For the different fiber volume fraction 0.3, 0.32, 0.34, 0.36, and 0.38, the in-plane thermal conductivity decreases by 2.7%, 2.8%, 2.9%, 2.5%, and 2.4% when the porosity φ_i increases from 0 to 0.01. This can be explained that the thermal conductivity of the air is smaller than that of the SiC. Besides, it is also concluded that the in-plane thermal conductivity decreases with the increase of the carbon fiber volume fraction. The reason is that the thermal conductivity of carbon fiber is smaller than that of the SiC matrix.

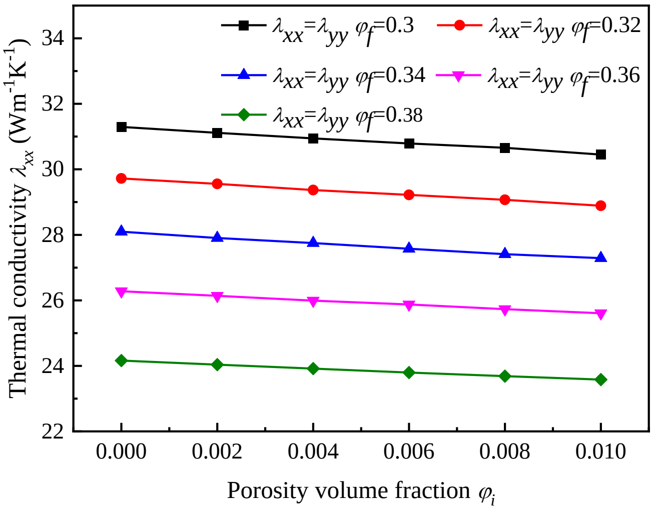

Figure 9. Relationship between in-plane thermal conductivity (λ_{xx}, λ_{yy}) and porosity inside the yarn φ_i with different carbon fiber volume fraction φ_f

According to the above analyses, the slight change in the porosity φ_i still causes the obvious change in the in-plane and out-of-plane thermal conductivity. Therefore, it is necessary to consider the porosity inside the yarn to predict the effective thermal conductivity of the composite.

3.3. Effect of the porosity outside the yarn on the thermal conductivity

Figure 10 shows the relationship between the out-of-plane thermal conductivity λ_{zz} and the porosity outside the yarn φ_o with different carbon fiber volume fractions φ_f. The porosity inside the yarn φ_i is taken as 0.006. It is concluded that the out-of-plane thermal conductivity decreases with the increase of the porosity φ_o At different carbon fiber volume fractions 0.3, 0.32, 0.34, 0.36, and 0.38, when the porosity φ_o increased from 0 to 0.25, the out of plane thermal conductivity decreased by 38.4%, 38.9%, 39.7%, 41.0%and 43.7% respectively. This can be explained that the thermal conductivity of the air is smaller than that of the SiC. From

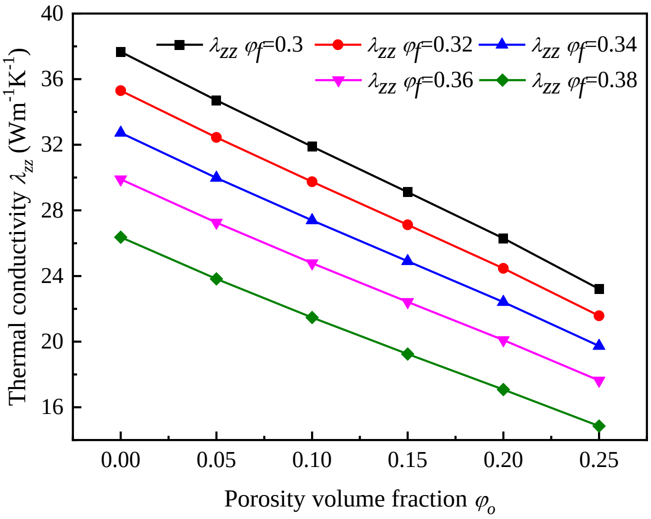

Figure 10. Relationship between out-of-plane thermal conductivity λ_{zz} and porosity outside the yarn φ_o with different carbon fiber volume fraction

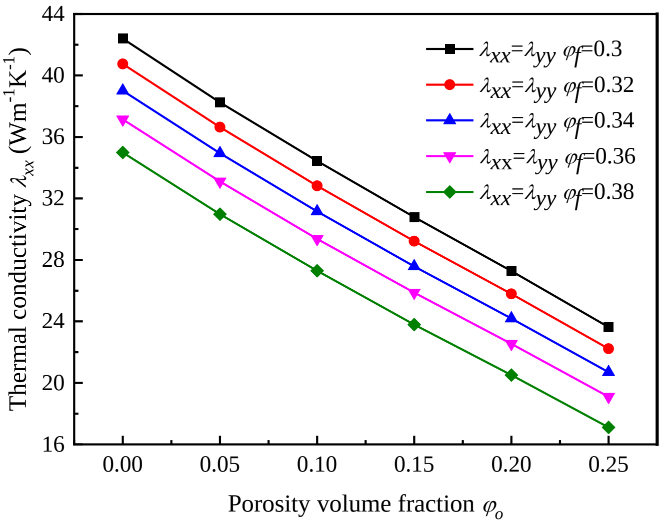

Figure 11. Relationship between the in-plane thermal conductivity (λxx, λyy) and the porosity outside the yarn φ_o with different carbon fiber volume fraction φ_f

Fig. 10, the study reaches the same conclusion shown in Fig. 8 that the out-of-plane thermal conductivity of the composite decreases with the increase of the carbon fiber volume fraction

Figure 11 shows the relationship between the in-plane thermal conductivity (λ_{xx}, λ_{yy}) and the porosity outside the yarn φ_o with different carbon fiber volume fractions φ_f. The porosity inside the yarn φ_i is equal to 0.006. The in-plane thermal conductivity decreases with the increased of the porosity φ_o. At different fiber volume fractions 0.3, 0.32, 0.34, 0.36, and 0.38, when the porosity φ_o increases from 0 to 0.25, the in-plane thermal conductivity decreases by 44.3%, 45.5%, 46.9%, 48.7%, and 51.1%. This can be explained that the thermal conductivity of the air is smaller than that of the SiC. Besides, the study reaches the same conclusion shown in Fig. 9 that the in-plane thermal conductivity of the composite decreases with the increase of the carbon fiber volume fraction.

4. Conclusions

In this work, the influence of carbon fiber volume fraction and yarn porosity on the effective thermal conductivity of C/SiC composite materials were studied. A unit cell model was established for 3DP C/SiC composite materials. Considering the influence of internal and external pores of the yarn, the effective thermal conductivity of the yarn along the in-plane and out of plane directions is analyzed. In addition, the effects of porosity and carbon fiber volume fraction on the effective thermal conductivity of composite materials were also studied. This numerical method is expected to provide direct guidance for designing composite materials with different porosity and fiber volume fractions. Based on the numerical results in this study, the research findings are as follows:

1) The effective thermal conductivity of composite materials gradually decreases with the increase of carbon fiber volume fraction and porosity. And the in-plane thermal conductivity is greater than the out of plane thermal conductivity.

2) The difference between in-plane thermal conductivity and out of plane thermal conductivity decreases as the external porosity of the yarn increases. For fiber volume fractions of 0.3, 0.32, 0.34, 0.36, and 0.38, an increase in yarn porosity from 0 to 0.01 results in decreases of 2.8%, 2.9%, 2.5%, and 2.4% in in-plane thermal conductivities, and decreases of 3.4%, 3.7%, 3.9%, 4.1%, and 4.0% in out-of-plane thermal conductivities, respectively. Therefore, it is necessary to consider the porosity inside the yarn to predict the effective thermal conductivities of the composites.

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Nomenclature

List of Symbols

a-length of the unit cell in *y* direction, [mm]
b-length of the unit cell in *x* direction, [mm]
c-height of the woven yarn, [mm]
d-diameter of the piercing yarn, [mm]
h-height of the unit cell, [mm]
q-heat flux, [Wm^{-2}]
r_1-radius of spherical pores inside the yarn
r_2-radius of spherical pores outside the yarn
S_x-spacing between two neighboring yarn in *x* directions, [mm]
S_y-spacing between two neighboring yarn in *y* directions, [mm]
T-Temperature, [K]
w-width of the woven yarn, [mm]

Greek symbols

λ_a-axial thermal conductivity of the yarn, [$Wm^{-1}K^{-1}$]
λ_t-transverse thermal conductivity of the yarn, [$Wm^{-1}K^{-1}$]
λ_{xx}, λ_{yy}, λ_{zz}-thermal conductivity in *x*, *y*, *z* directions, [$Wm^{-1}K^{-1}$]
φ_f-carbon fiber volume fraction of composites
φ_i-porosity inside the yarn of composites
φ_o-porosity outside the yarn of composites

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