



Sharif University of Technology
Scientia Iranica
Transactions B: Mechanical Engineering
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2D hierarchical heat transfer computational model of natural fiber bundle reinforced composite

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Received 13 September 2014; received in revised form 18 November 2014; accepted 12 April 2015

KEYWORDS

Hierarchical composite;
 Natural fiber bundle;
 Lumen;
 Heat conduction;
 Finite element method;
 Thermal conductivity.

Abstract. In this paper, a two-dimensional (2D) hierarchical computational model was developed for analysis of heat transfer in unidirectional composites filled with a doubly periodic natural fiber bundle. The reinforcement in the composite encloses a large number of small lumens, which hints that the composite, consisting of matrix and natural fiber bundles, involves structures at several level scales. In the model, the unit Representative Volume Element (RVE) of the composite, with fibers arranged periodically, was taken into consideration and equivalent models were converted from differently scaled RVEs by a two-step homogenized procedure. Subsequently, numerical simulation of the heat-transfer process in each model was performed by finite element analysis and the overall transverse thermal conductivity of each model was obtained numerically. To verify the developed composite models, an optional interrelationship between the overall thermal conductivity of the equivalent natural fiber bundle and the solid region phase in it was obtained for the first-step homogenization and was then compared with analytical or numerical results from other methods. Finally, a sensitivity analysis was conducted with the models to investigate how changes in the values of important variables, such as thermal conductivity and volume fraction of the constituent, can affect the effective thermal properties of the composite.

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1. Introduction

As early as 3000 B.C., mud filled with plant stems has been used to construct buildings. This can be viewed as a prototype of modern natural fiber reinforced composites, which are an emerging area in composite science. Currently, natural fibers, including kenaf, hemp, bamboo fibers etc., are environmental friendly low cost fibers compared to conventional man-made solid fibers like carbon and glass fibers, and have low density and high specific properties. More importantly, they are biodegradable. Due to the special features of natural fibers, composites reinforced with them, such

as natural fiber reinforced polymer/cement composites, have been viewed as green and environmental friendly materials and, thus, have been widely accepted for engineering applications [1-3]. As one of the inherent characteristics of natural fiber is its microstructure, its excellent thermal insulating property has shown great potential for the development of new green and energy-saving composites. It was suggested that the moisture content, thickness, internal air cavities and surface structuring of bark can significantly affect flame retardancy and heat insulation of wood [4]. Liu et al. revealed that natural hemp fibers, consisting of cellulose or lumens, can present lower thermal conductivity [5]. Considering the high and increasing cost of energy harvesting and the ecological hazards of over consumption of energy, studying the thermal properties of natural fiber or composites filled with it is becoming an ever

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important issue. Current research includes experimental investigation of the influence of fiber content on the mechanical and thermal properties of kenaf fiber reinforced thermoplastic polyurethane composites [6], pineapple leaf fiber reinforced composites [7], hemp fiber reinforced composites [8], finite element simulation and analytic modelling the transverse thermal conductivity of Manila hemp fiber in solid regions [5], PLA-bamboo fiber composites [9], the temperature profile and curing behavior of hemp fiber/thermoset composite during the molding process [10], and the effect of the microstructure of natural fiber on the transverse thermal conductivity of unidirectional composite filled with natural fibers [11]. Additionally, Srinivasan et al. tested the mechanical and thermal performance of polymer composites filled with banana and flax fibers, whose cellulose content, respectively, are 63% and 71% [12]. Zheng numerically investigated the anisotropic thermal conductivity of natural fiber bundles with lumens, and the results showed that the large number of lumens in the fiber bundle can induce approximate isotropy [13]. All the work mentioned above is of great benefit regarding the understanding of the thermal transfer mechanism in natural fiber. However, these research works considered the fiber reinforced composite as a whole, or only studied the fiber microstructure itself. The answer to questions as to how the microstructure affects thermal conduction of bulk composite properties is yet unknown, which is critical in guiding the design of natural fiber filled composites with desirable thermal properties.

Hierarchical structures are exhibited in many natural and man-made materials. Analysis based on different hierarchical levels is expected to give a deep understanding of the relationship between microstructures and the physical properties of composites. The hierarchical order of a structure or a material may be regarded as the number of levels of scale with a recognized structure [14]. At each level of the structural hierarchy, one may model the material as a continuum for the purpose of analysis. Such an assumption is warranted if the structure size at each level of the hierarchy is significantly different. Taking hemp fiber bundle reinforced composites, as an example, we study the bulk thermal properties of the composites affected by the inherent microstructure of fiber bundles via hierarchical structuring. In such a natural fiber bundle, there are a large number of lumens filled with air in their transverse directions (see the cross-section morphology of the hemp fiber bundle in [5] for details). The thermal properties of the natural fiber bundle may vary considerably depending on the volume and size of the lumens and the thermal property of the solid region encircling the lumen walls. Figure 1 shows a schematic illustration of a three-level hierarchy composite model, with each natural fiber

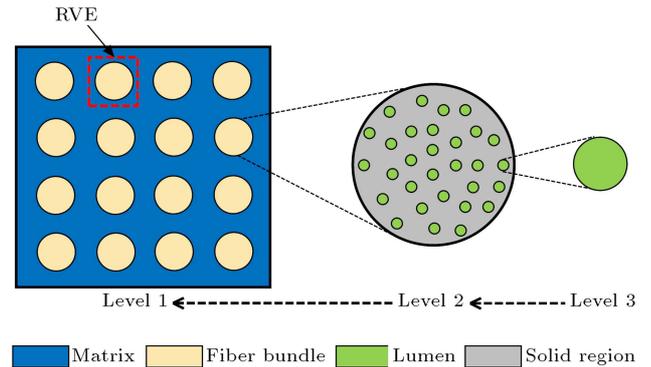


Figure 1. Schematic view of three-level hierarchy model of doubly periodic natural fiber bundle reinforced composites.

bundle consisting of lumens and a solid region. It is observed that the large-scale fiber bundle (i.e. about $200 \mu\text{m}$ for a hemp fiber bundle) is filled with many small-scale lumens (i.e. about $16.5 \mu\text{m}$ for lumen) in the solid region [5]. As such, an entire fiber bundle is regarded as a composite consisting of lumen fillers and a solid region phase. This allows us to analyze the thermal property hierarchically and use equivalency to bridge models between different scales. In this paper, a 2D hierarchical finite element model of a natural fiber bundle composite is established to investigate the influences of the microstructure of natural fiber bundles to the bulk thermal property of the composite [15]. A computational model is also employed to determine the optional interrelationship between the thermal properties of the solid region and the fiber bundle for the purpose of verification. Heat transfer in the natural fiber bundle reinforced composite is analyzed based on the Finite Element Method (FEM) [16,17], implemented by the commercial software ABAQUS. To verify the present composite model, the effects of the thermal property of the solid region phase on the equivalent thermal property of the fiber bundle are analyzed using the finite element model [18–20]. Then, an optional interrelationship of thermal properties between them is established by a curve fitting technique [21] to give a fast and accurate prediction of the material properties of both the fiber bundle and the composite as a whole. Further, a sensitivity analysis is conducted to investigate how value changes of important parameters, including thermal conductivity and volume fraction of the constituents, can affect the overall thermal properties of the composite.

2. 2D hierarchical finite element model of natural fiber bundle reinforced composite

When the composite of interest has a doubly periodic distribution of fibers or fiber bundles, a unit Representative Volume Element (RVE) or cell of the composite

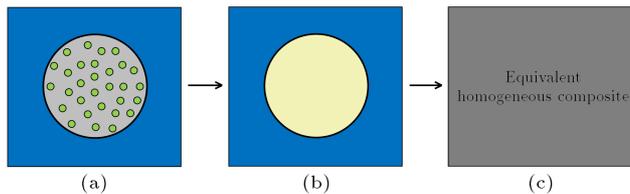


Figure 2. A two-step homogenized procedure for the natural fiber bundle reinforced composite: (a) Original RVE; (b) first equivalent RVE; and (c) second equivalent RVE.

can be adopted as the basic element. Then, two equivalent models in different size scales are converted by two-step homogenized procedures for heat-transfer analysis. The fiber bundle is assumed to be embedded into a square matrix phase like polymer, concrete, etc., to form a RVE composite system, as shown in Figure 2(a), including the matrix phase, lumen phase and solid region phase. Adjacent material phases are assumed to be bonded perfectly. In this schema, the fiber bundle is usually long enough in comparison to its cross section dimensions, so that the model is assumed to be infinite in the longitudinal direction. Moreover, theoretically, the distribution of the lumens will cause the anisotropy of the composite under consideration. In fact, the anisotropy of the composite becomes weak with the increasing number of lumens [5]. This means that when the number of lumens is large enough, the effect of the distribution of lumens tends to be isotropy. Here, we assume an isotropic thermal property of the fiber bundle for the case with a large number of lumens.

A two-step homogenization procedure is used here for thermal property calculation of the composite model, as shown in Figure 2. Firstly, the fiber bundle, consisting of large number of lumens, is homogenized to produce an equivalent material phase (see Figure 2(b)). This material phase is then considered as a reinforcement of the matrix in the transverse direction. The homogenization of this new composite model, as shown in Figure 2(b), gives the final equivalent homogeneous material phase, as displayed in Figure 2(c).

In order to determine the effective thermal property of the composite, proper boundary conditions should be prescribed to the RVE, as has been undertaken by many researchers in the analysis of heterogeneous materials [22–27]. Islam and Pramila [23] suggested that in heat-transfer analysis, the prescribed temperature boundary conditions on the parallel boundaries of the rectangular RVE can produce the most accurate results up to a relatively high fiber volume fraction. Thus, in the computing model displayed in Figure 3, two different temperatures, T_1 and T_0 , are specified on its vertical edges, and the remaining top and bottom edges are assumed to be insulation. It is assumed that $T_1 > T_0$, so that the horizontal heat flux loaded on the left side face (data-

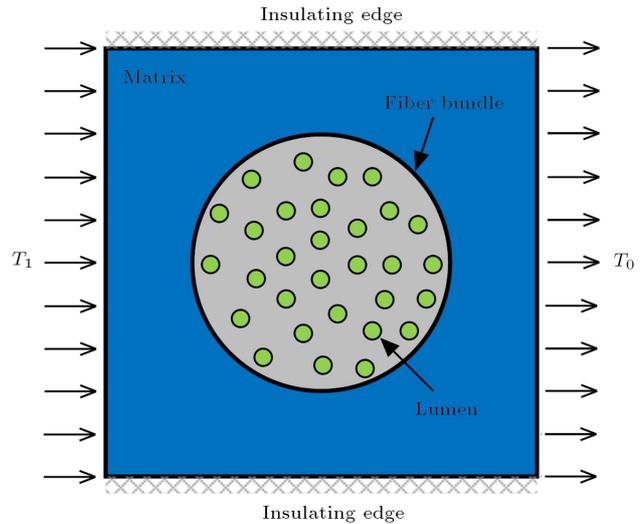


Figure 3. Schematic illustration of a square cell embedded with natural fiber bundle containing lumens.

collection surface) is positive. For instance, in practical computation, we can let $T_1 = 20^\circ\text{C}$ and $T_0 = 0^\circ\text{C}$.

According to Fourier's law of heat transfer in isotropic media, we have:

$$q_1 = -k \frac{\partial T}{\partial x}, \quad q_2 = -k \frac{\partial T}{\partial y}. \quad (1)$$

The effective thermal conductivity of the composite, k_e , can then be evaluated by [23,28]:

$$k_e = \frac{QL}{(T_1 - T_0)}. \quad (2)$$

In Eqs. (1) and (2), T is the temperature change in the Cartesian coordinate system, x – y , and k is the thermal conductivity of the isotropic material. Q stands for the average value of the heat flux component, q_1 , loaded on the left side face of the cell, which can be evaluated by trapezoidal numerical integration. L is the side length of the cell.

In our analysis, the side length of the RVE or cell used is assumed to be 1, which is a normalized length. Furthermore, the volume fraction of the lumens to the fiber bundle is assumed to be a constant of 30.87%, which is an actual experimental value of the Manila hemp fiber bundle [5]. The volume fraction of fiber bundle to composite is initially set to be a constant of 50%, a relatively high volume concentration, unless otherwise specified. The thermal conductivity of the matrix is taken to be 0.42 W/(mK), which corresponds to the polymer matrix [8]. According to the known research results [4], the anisotropy of the fiber bundle becomes smaller as the number of lumens in it increases, and then, the composite tends to isotropy. Here, since there is no available data on the number of lumens in a fiber bundle in the literature,

it is assumed to be 106, which is close to the actual dispersion of lumens in the fiber bundle (see the cross-section morphology of the hemp fiber bundle in [4] for details) and is also enough to produce the isotropic thermal property of the fiber bundle and the composite. Besides, the thermal conductivities of a composite, matrix and solid region are, respectively, normalized, with respect to those of lumen, that is, 0.026 W/(mK), in the following post-processing of numerical results. Finally, to simplify the analysis, symbols k_m , k_{fb} , k_s and k_l denote, respectively, the thermal conductivity of the matrix, the equivalent fiber bundle, the solid region and lumen, and v_{fb} and v_l , respectively, stand for the volume fraction of the fiber bundle and the lumen.

3. Numerical experiments

3.1. Verification of the present computational composite model

As mentioned in the introduction, two composite models, including the original RVE and the first equivalent RVE, are here investigated, respectively, using the finite element method, with which the bulk thermal conductivities of composites are calculated. Then, an optional relationship of thermal conductivity between the solid region and the fiber bundle is derived by curved fitting to verify the present computational composite model.

3.1.1. Computational analysis of the original composite model

To conduct finite element analysis, the original composite model with 106 internal lumens, as shown in Figure 4(a), is discretized by a total of 51680 quadratic elements, with 155841 nodes (see Figure 4(b)), generated by ABAQUS. In order to determine the dependence of the thermal conductivity of the composite on that of the solid region, it is assumed that the normalized thermal conductivity of the solid region changes in the range [1,10], which corresponds to the variation from poorly conducting to highly conducting. By means of finite element analysis, distribution of the horizontal

heat flux component, q_1 , on the data-collection surface can be determined. Then, its corresponding average value, Q , can be evaluated by trapezoidal numerical integration for each specific value of the normalized thermal conductivity of the solid region. Subsequently, the overall thermal conductivity of the composite is obtained using Eq. (2).

From the computational model, the contour plots of normalized temperature and horizontal heat flux components in the entire composite domain under consideration are, respectively, obtained and displayed in Figures 5 and 6 (for the case of $k_s/k_l = 1$ and $k_s/k_l = 5$) to demonstrate the effect of thermal conductivity in the solid region on the heat transfer performance in the composite. It is obvious that heat is transferred into the fiber bundle from left to right through thermal conduction. When $k_s/k_l = 1$, the thermal conductivity of the solid region and lumen becomes identical. Thus, just a smaller portion of heat passes through the fiber bundle, while a greater portion of it passes around the fiber bundle, due to the low thermal conductivity of lumen. However, for the case $k_s/k_l = 5$, the solid region has a larger thermal conduction capacity than that of the lumen, so, more heat flows into the fiber bundle and passes through the solid region. The mismatch of thermal property between the solid region and the lumen significantly increase the quantity of the heat flux component in the fiber bundle. Besides, in either case, the process of heat transfer in the composite becomes longer and more complicated, leading to reduction in the thermal properties of the composite. Furthermore, Figure 7 displays the variation of the normalized effective thermal conductivity of the composite in terms of the thermal conductivity of the solid region. Results in Figure 7 show that the simulated effective thermal conductivity of the composite increases with an increase in the value of the thermal conductivity of the solid region. Simultaneously, it is obvious that variation of the overall thermal conductivity of the composite exhibits slight nonlinearity. To model this change, we use a quadratic polynomial fitting curve:

$$\frac{k_e}{k_l} = -0.008432 \left(\frac{k_s}{k_l} \right)^2 + 0.5236 \left(\frac{k_s}{k_l} \right) + 5.673. \quad (3)$$

This is used to establish the approximated relationship of thermal conductivity between the solid region and the fiber bundle.

3.1.2. Computational analysis of the first equivalent composite model

Here, the first equivalent composite model, shown in Figure 8(a), is taken into consideration to investigate the effect of the equivalent fiber bundle on the composite. In the model, the practical fiber bundle is homogenized as a homogeneous material

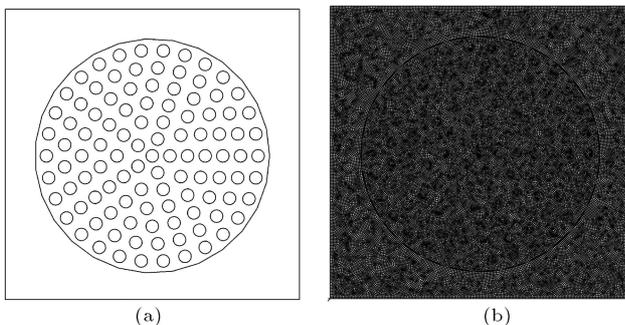


Figure 4. Finite element model of RVE of natural fiber bundle composites including 106 lumens: (a) Computational domain; and (b) computational mesh.

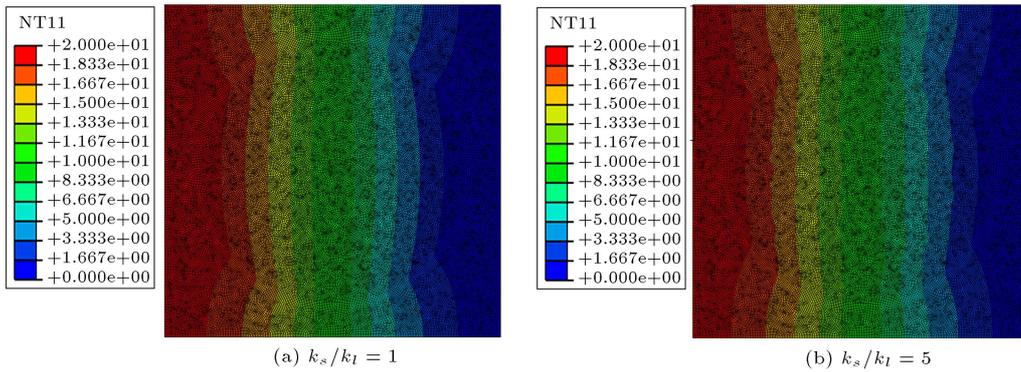


Figure 5. Distribution of temperature in the computational domain.

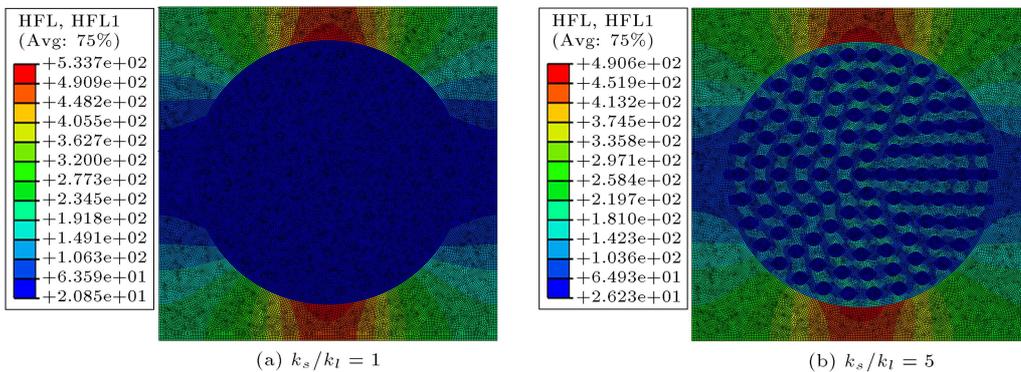


Figure 6. Distribution of horizontal heat flux component in the computational domain.

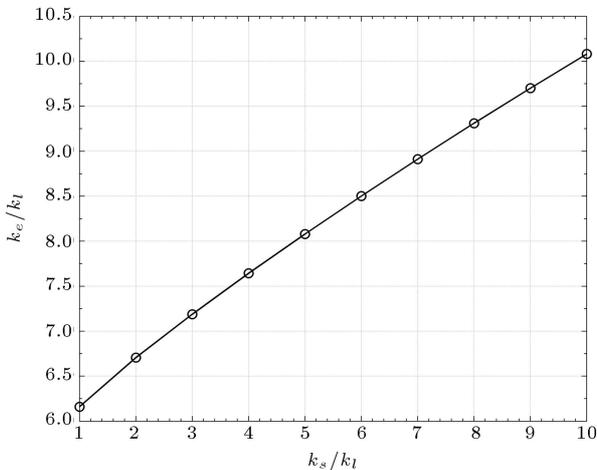


Figure 7. Variation of the effective thermal conductivity of the composite against that of the solid region.

with equivalent material property, and is replaced with a solid fiber of the same size for computation, as shown in Figure 2(b). The same boundary conditions as those applied in the original composite model, as shown in Figure 3, are employed. To carry out finite element simulation, 12247 quadratic quadrilateral heat transfer elements generated by ABAQUS are used to discretize the first equivalent composite domain. To investigate the variation of the thermal property of the composite caused by the homogenized fiber bundle, we

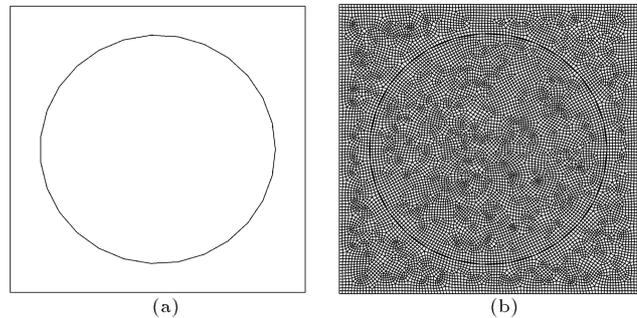


Figure 8. Finite element model of the first equivalent RVE: (a) Computational domain; and (b) computational mesh.

assume that the normalized thermal conductivity of the homogenized fiber bundle changes in the interval [1,10]. Thus, we can obtain a curve to describe the dependence between the equivalent fiber bundle and the composite. Numerical results in Figure 9 show that the simulated thermal conductivity of the composite increases with an increase in the value of the thermal conductivity of the equivalent fiber bundle, as expected. Also, a weak nonlinear variation is observed in Figure 9. Fitting the numerical results in Figure 9 by polynomial approximation yields:

$$\frac{k_c}{k_l} = -0.01486 \left(\frac{k_{fb}}{k_l} \right)^2 + 0.8932 \left(\frac{k_{fb}}{k_l} \right) + 5.301. \quad (4)$$

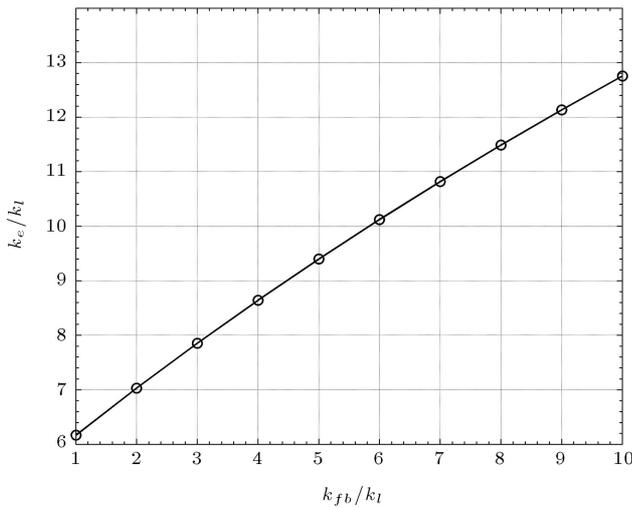


Figure 9. Variation of the effective thermal conductivity of the composite against that of the equivalent fiber bundle.

3.1.3. Relationship of thermal conductivity between the solid region and the fiber bundle

The equivalence of the two composite models, shown, respectively, in Figures 4(a) and 7, requires the same effective thermal conductivity of the composite under the same boundary conditions. Therefore, combining Eqs. (3) and (4), one can get an optional relationship of thermal conductivity of the fiber bundle and the solid region, that is:

$$\begin{aligned}
 & -0.01486 \left(\frac{k_{fb}}{k_l} \right)^2 + 0.8932 \left(\frac{k_{fb}}{k_l} \right) \\
 & = -0.008432 \left(\frac{k_s}{k_l} \right)^2 + 0.5236 \left(\frac{k_s}{k_l} \right) + 0.372, \quad (5)
 \end{aligned}$$

from which, the variation of k_s , with respect to k_{fb} , is plotted in Figure 10.

To verify the obtained relation of thermal conductivities between the solid region and the fiber bundle, an analytical solution, taken from the Hasselman-Johnson’s model [5,29], is employed for comparison. Here, the analytical expression of the thermal conductivity of the solid region, k_s , with respect to that of the fiber bundle, k_{fb} , is written as:

$$\frac{k_s}{k_l} = 0.9465 \left(\frac{k_{fb}}{k_l} - 1 \right) + \sqrt{0.8960 \left(\frac{k_{fb}}{k_l} - 1 \right)^2 + \frac{k_{fb}}{k_l}}, \quad (6)$$

with $v_l = 30.87\%$. Note that Eq. (6) is different from that in reference [5]. For the purpose of comparison, we plot Eq. (6) in Figure 10. Especially, if k_{fb} is 0.115 W/(mK) [5,8]; k_s can be calculated from Eq. (6) and has value of 0.1847 W/(mK).

In Figure 10, it is observed that there is good agreement between the quadratic fitting curve and

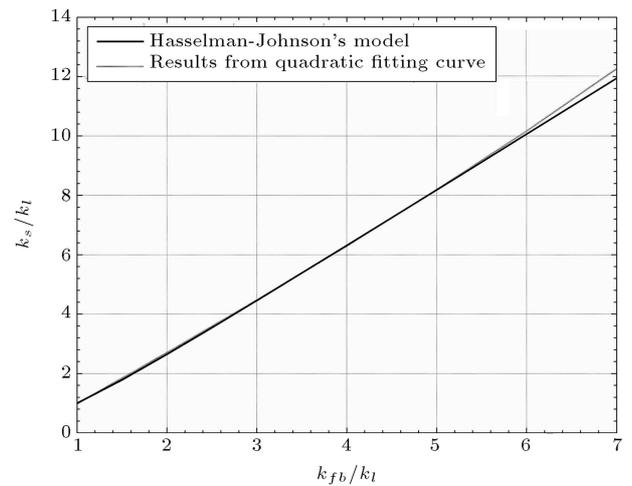


Figure 10. Approximated relation of thermal conductivities of the natural fiber bundle against the fiber solid region.

the theoretical curve. For example, when $k_{fb} = 0.115$ W/(mK), k_s from the fitting curve Eq. (5) is 0.1843 W/(mK), which has a relative deviation of 0.21% compared to the theoretical solution of 0.1847 W/(mK) (obtained from Eq. (6)). In research work [5], the evaluated value of k_s is 0.1849 W/(mK). Therefore, the present computational composite model on the fiber bundle, including numbered lumens, has been verified and the obtained quadratic relationship between the thermal conductivity of the solid region and the fiber bundle can be used to estimate the thermal conductivity of the natural fiber or the solid region, if one of them is known.

Besides, from Figure 10, it is clear to see that the existence of lumens significantly weakens heat transfer in the fiber bundle, and then decreases the thermal conductivity of the equivalent fiber bundle, k_{fb} , in the first equivalent RVE. As a result, k_{fb} must be less than k_s , significantly, which can be seen from Figure 10.

3.2. Sensitivity analysis

A sensitivity analysis is carried out in this section. The purpose of a sensitivity analysis is to identify individual or a combination of parameters that may affect the effective thermal conductivity of the composites. This is important since accurate prediction of the effective thermal conductivity of composites may significantly benefit their design.

The parameters examined here include the volume fraction of the fiber bundle to the matrix, the volume fraction of the lumen to the fiber bundle, and the thermal conductivity of the matrix. To investigate how changes in each of these parameters may affect the effective thermal conductivity of the composite, serial values that are different from practical values are considered, i.e. some values are higher than the practical value and others may be lower.

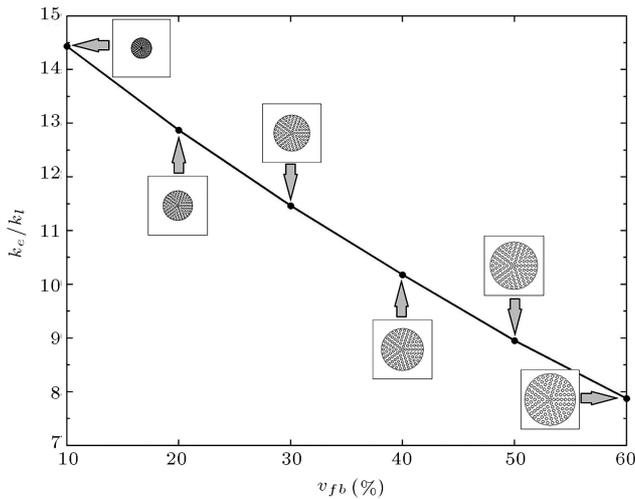


Figure 11. Variation of the effective thermal conductivity of the composite against the volume fraction of the fiber bundle.

3.2.1. Effect of volume fraction of the fiber bundle

Let us begin by considering the influence of the volume fraction of the fiber bundle on the effective thermal conductivity of the composite. In the analysis, the volume fraction of the lumen to the fiber bundle is assumed to be a constant of 30.84%. Figure 11 presents the variation of the normalized thermal conductivity of the composite, k_e/k_l , in terms of the volume fraction of the fiber bundle, v_{fb} . It can be seen that there is a considerable decrease of k_e/k_l when v_{fb} increases. The average value of the decrease of k_e/k_l is 1.312 for every 10% increase in the value of v_{fb} .

3.2.2. Effect of lumen volume fraction to the fiber bundle

The influence of the volume fraction of the lumen on the effective thermal conductivity of the composite is investigated in this section. In the analysis, the volume fraction of the fiber bundle to the composite is assumed to be 50%. Alteration of the volume fraction of the lumen is fulfilled by changing the radius of the lumen. Figure 12 displays the variation of the normalized thermal conductivity of the composite, k_e/k_l , in terms of the volume fraction of the lumen, v_l . It can also be seen that there is a considerable decrease of k_e/k_l with an increase of v_l . In this case, the volume fraction of the lumen increases by 10%, and the normalized effective thermal conductivity will decrease about 0.538. In contrast to the volume fraction of the fiber bundle, the change of the volume fraction of the lumen has less influence on the effective thermal property of the composite.

3.2.3. Effect of thermal conductivity of the matrix

Finally, the effect of thermal conductivity of the matrix on the effective thermal property of the composite is investigated and the numerical results are displayed in

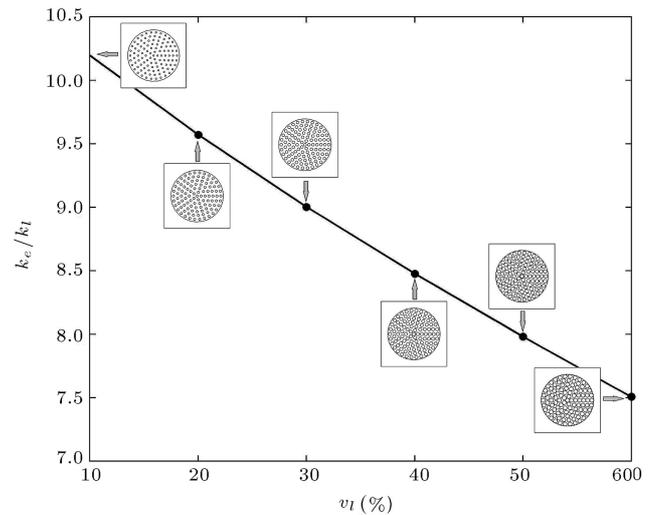


Figure 12. Variation of the effective thermal conductivity of the composite against the volume fraction of the lumen.

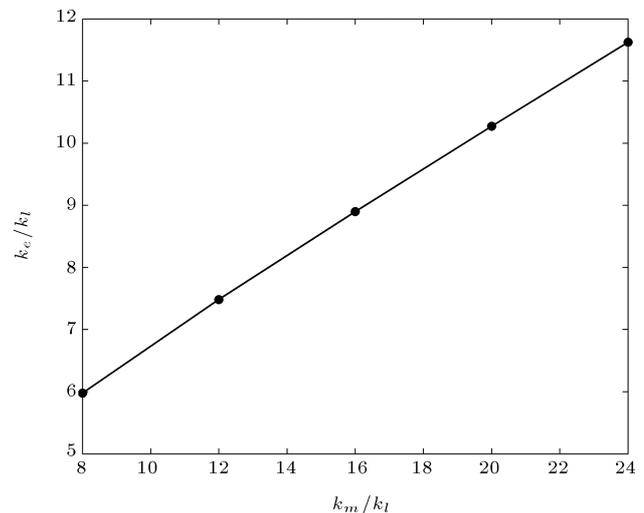


Figure 13. Variation of the effective thermal conductivity of the composite against the thermal conductivity of the matrix.

Figure 13. In the computation, the volume fractions of the fiber bundle and the lumen are taken as 50% and 30.87%, respectively. It can be seen from Figure 13 that there is a remarkable increase of k_e/k_l with the increase of k_m/k_l , and when the normalized thermal conductivity of the matrix increases by 1, the normalized effective thermal conductivity will increase about 0.353. Compared to the numerical results in Figure 7, which depict the effect of thermal conductivity of the solid region in the fiber bundle on the effective thermal conductivity of the composite, it is found that the solid region has a larger influence than the matrix on the effective thermal property of the composite. The main reason is that the larger volume fraction of the fiber bundle dominates thermal transfer behavior in the composite.

4. Conclusion

In this paper, a 2D hierarchical computational model of the heat transfer of unidirectional composites filled with a natural fiber bundle was developed and then verified by comparison with the analytic Hasselman-Johnson's results and other numerical results. Subsequently, a sensitivity analysis was conducted to investigate the effects of the thermal conductivity of the solid region and the matrix, and volume fractions of the fiber bundle and lumen on the entire thermal conductivity of the composite. Numerical results show that the bulk thermal property of the composite decreases with an increase in the volume fraction of both the fiber bundle and the lumen. The volume fraction of the fiber bundle has a more significant influence on the effective thermal property of the composite than the volume fraction of the lumen. Moreover, the bulk thermal property of the composite increases with an increase in the thermal properties of both the matrix and the solid region. For the case of a larger volume fraction of fiber bundle, the increase of thermal conductivity of the solid region produces the larger effective thermal conductivity of the composite than that of the matrix.

Besides, the present computational method is also applicable for evaluating the thermal conductivity of composites filled with other bundled natural fibers containing a large number of lumens, such as kenaf core fiber.

Acknowledgements

The research work is partially supported by the Natural Science Foundation of China (Grant no. 11102059; 11472099) and the Creative Talents Program of Universities in Henan Province (Grant no. 13HASTIT019).

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