Random modeling for transverse thermal conductivity in unidirectional silica/phenolic composite

Guiliang Dai[#]

[#] No. 1 Middle School of Bayingol Mongolian Autonomous Prefecture, Korla 841000, Xinjiang Uygur Autonomous Region, P.R. China

Abstract *The purpose of this work was to study the influence of microstructure on effective transverse thermal behavior of unidirectional silica fiber reinforced composites with carbonized phenolic resin matrix. The randomly distributed fiber model is firstly established and then the temperature dependent thermal conductivity of silica fiber and phenolic matrix is taken into account for predicting the effective thermal conductivity of composite. Results provided by finite elements simulations for the silica/phenolic composite of interest have shown that the random model can give closer predictions to the theoretical results from Maxwell model.*

Keywords — *Thermal conductivity, silica fiber, phenolic matrix, unidirectional composite, randomness*

I. INTRODUCTION

Unidirectional fiber reinforced composites made of long fibers and matrix have been used for most engineering applications [1, 2]. Among them, silica/phenolic composite is typically used in aerospace applications as ablative material, which is made of silica fiber fabrics and phenolic resin matrix [3, 4]. For ablative materials, the lower the thermal conductivity, the better the thermal insulation performance. Therefore, it is interesting to predict the thermal conductivity of silica/phenolic composite in order to better study the heat transfer performance of it. To do this, it is necessary to develop effective models to predict the overall thermal conductivity precisely.

Considering the microstructure, the silica fiber is usually dispersed in the phenolic matrix in random mode. Therefore, how to assess the influence of randomly dispersed fibers to the effective thermal properties of composites have to be paid more attention recently [5, 6]. For example, the influence of interphase in the unidirectional composites with randomly distributed fibers was studied by the fast Fourier transforms simulation [7]. The non-circular fiber was also considered for the assessment of orientation effect of fiber [8]. Additionally, the cluster behavior of fibers in unidirectional composites was investigated and the results revealed that the fiber cluster has little influence for the composites, especially with low fiber volume fraction [9, 10]. Besides, the efficient numerical models based on hybrid finite element theory were developed for simulating the thermal and mechanical properties of unidirectional composites [11-14]. Therefore, in order to accurately predict the properties of unidirectional composites, it is necessary to develop the proper micro-scale composite model which can simultaneously take into account the influence of controlling parameters.

The overall objective of this paper is to perform a comparative investigation between the numerical and theoretical predictions for the effective transverse thermal conductivity of unidirectional silica/phenolic composite. The numerical prediction is numerically evaluated by finite element simulation followed by an area averaging of local thermal properties for the random fiber model established by a simple random fiber generation algorithm, while the theoretical prediction is obtained by four empirical formulas. The computational model is assessed and conclusions are summarized and proposed for guiding the design of the silica/phenolic composite.

II. MODELING METHODOLOGY

A. Randomly distributed fiber model

For an unit cell of unidirectional fiber-reinforced composite including multiple randomly distributed fibers, the relation of the fiber volume fraction v_f, the number of fibers n_f, the fiber size (radius) r_f and the unit cell size (side length) a can be written as

$$v_f = \frac{n_f \times \pi r_f^2}{a \times a} \tag{1}$$

from which one can have

$$a = r_f \sqrt{\frac{n_f \times \pi}{v_f}} \tag{2}$$

Generally, the fibers are randomly dispersed in the matrix. Thus, it is desired to include as many fibers as possible in the micromechanical unit cell model to better reflect real fiber configuration at the microscale level. To establish the micromechanical unit cell model with random fiber array, it is important to assume that (1) the overlap of fibers is not permitted; (2) fibers locate in the unit cell; (3)

fibers are allowed to intersect with the cell boundary to satisfy the periodical requirement of temperature field. Under these assumptions, the random fiber array can be generated by the random fiber generation algorithm, which is regarded as the closest representation to the real case [7, 15, 16]. In the implementation of the random fiber generation algorithm, the input parameters include fiber size, fiber quantity and fiber volume fraction, from which the cell size can be evaluated by Eq. (2). Then the new fiber can be put into the cell randomly if it doesn't coincide with the existed fibers generated in the previous step until the specific fiber quantity reaches. Specially, when the fiber intersects with the cell boundary edge, the fiber cross-section will be cut by the edge and the cutting out part of the fiber should be supplemented in the opposite edge to keep the periodic characteristics of the geometrical model. Following this rule, the required two-dimensional composite geometrical model can be generated directly as shown in Fig. 1, in which $v_f = 56.1\%$, $n_f = 50$, and $r_f = 2.355$ μm, which corresponds to the silica fiber [4].

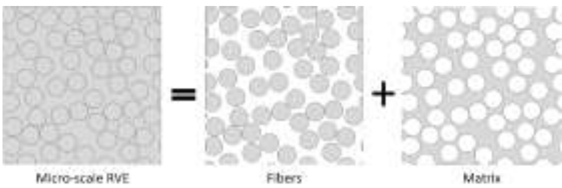

Fig. 1 Geometrical models of composites consisting of randomly distributed fibers and matrix

B. *Material properties*

The material studied is the carbonized silica/phenolic composites, which is composed of the high silica fiber and the carbonized phenolic resin matrix. Their thermal conductivities are temperature-dependent and thus are summarized in Table 1 at different environmental temperatures ranging from 100℃ to 800℃ [3, 4].

TABLE 1
Thermal conductivity of constituent materials of composite at different environmental temperatures

Temperature (℃)	100	200	300	400	500	600	700	800
Matrix (W/m/K)	3.368	3.847	4.143	4.397	4.548	4.682	4.354	4.108
Fiber (transverse) (W/m/K)	0.383	0.431	0.433	0.447	0.462	0.481	0.579	0.675

C. *Boundary conditions*

In order to accurately simulate the heat transfer behavior of the composite, the boundary conditions are applied to the RVE in finite element analysis. In the steady-state thermal analysis, temperature is the only degree of freedom in the simulation. The left and right surfaces with different temperatures (T_1 and T_2) are set as the heat source and the heat sink. The other two surfaces are set as adiabatic surfaces due to the symmetry of the RVE. Thus, the effective thermal conductivity k_c of RVE can be calculated by

$$k_c = \tilde{q}a/(T_1 - T_2) \quad (3)$$

where $\tilde{q}$ is the averaged heat flow density on the surface perpendicular to the direction of heat flow. In practice, the averaged heat flow density can be evaluated by

$$\tilde{q} = \sum_{e=1}^{N} q_e A_e \Big/ \sum_{e=1}^{N} A_e \quad (4)$$

where N is the total number of elements in the unit cell, q_e and A_e are the centroid heat flow density and the area of the element e, respectively.

III. THEORETICAL MODELS

An extensive theoretical models for predicting the effective thermal conductivity of two-phase composites, i.e. fiber-reinforced composites, from literature is reviewed in this section. For two-phase composites, the Parallel and Series models define the upper and lower bounds of the effective thermal conductivity of composite, because these two models assume two extreme structure arrangements that the dispersed phases are in parallel or series along the heat transfer direction [4]. The Pilling et al. derived the semi-empirical formula for calculating the out-of-plane effective thermal conductivity of carbon fiber/epoxy resin composites based upon analogies in elasticity [17]. Maxwell was the first to study the effective thermal conductivity of polymer composites containing irregularly dispersed fillers by combining the potential theory and the Laplace equation [18].

- Parallel model

$$k_c = v_f k_f + (1 - v_f) k_m \quad (5)$$

- Series model

$$k_c = \frac{1}{v_f / k_f + (1 - v_f) / k_m} \quad (6)$$

- Pilling model

$$k_c = k_m \frac{(1 - v_f) k_m + (1 + v_f) k_f}{(1 - v_f) k_f + (1 + v_f) k_m} \quad (7)$$

- Maxwell model

$$k_c = k_m \frac{(k_f + 2k_m) + 2v_f (k_f - k_m)}{(k_f + 2k_m) - 2v_f (k_f - k_m)} \quad (8)$$

IV. THEORETICAL MODELS

A. *Finite element mesh*

In the simulation, the 3-node linear heat transfer triangular elements (DC2D3 in ABAQUS) are employed to model the computational domain, including the fiber region and the matrix region. To achieve the convergent results, the extremely fine mesh is used in this study. For the fiber region, the total number of elements are 50836 with 27576 nodes, while for the matrix region, the total number of elements are 36456 with 20195 nodes. Fig. 2 and Fig. 3 display the related finite element mesh in the fiber and matrix regions, respectively.

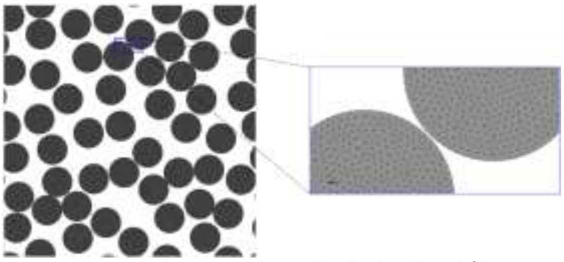

Fig. 2 Mesh division in the randomly distributed fibers

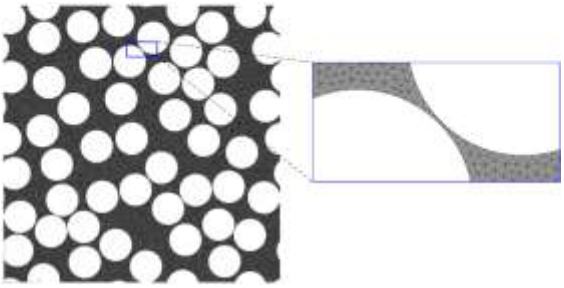

Fig. 3 Mesh division in the matrix region

B. Comparison of theoretical and numerical predictions

On the one hand, the temperature and transverse heat flux distributions in the micro-scale RVE are shown in Fig. 4. It is found that both the temperature and the transverse heat flux distribution become significantly uneven in the composite due to the existence of fibers in the matrix and the complex arrangement of them, and such nonuniformity is found to be mainly concentrated in the matrix region around the fiber. This is because the thermal conductivity of matrix is remarkably greater than that of fiber for the carbonized silica/phenolic composites under consideration.

On the other hand, by comparing the formula results with the simulation results in Fig. 5 at various temperature conditions, it is found that there is no formula which can match accurately. Among all models, Maxwell model gives better agreement to the FEM result than Pilling model, especially for the case that the environmental temperature is no greater than 600℃. Besides, as expected, all other predictions locate between the Parallel and Series models. Therefore, these two models can be used as the upper and lower limits of the fitting result.

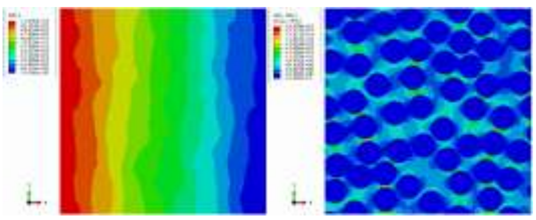

Fig. 4 Distributions of temperature and heat flux component q in the width direction in the micro-scale unit cell

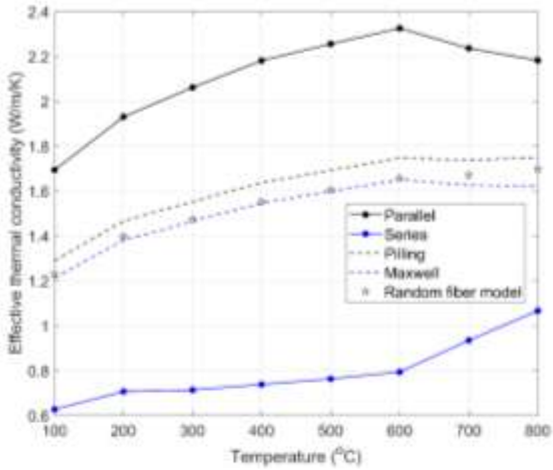

Fig. 5 Comparison of composite thermal conductivity at various temperatures

V. CONCLUSIONS

In this paper, the effective thermal conductivity of carbonized silica/phenolic composites under different environmental temperatures is predicted by the empirical formulas and the finite element simulation, which is carried out in a micro-scale representative unit cell with random fiber array. The fiber volume fraction is taken as 56.1%. It is found that the heat flux distribution becomes extremely uneven due to the significant mismatch of thermal property of the silica fiber and the carbonized phenolic matrix. Also, the comparison reveals that Maxwell model give more fitting predictions to the finite element results.

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