A NOVEL DETERMINATION OF THE MINIMAL SIZE OF A PROBABILISTIC REPRESENTATIVE VOLUME ELEMENT FOR FIBER-REINFORCED COMPOSITES' THERMAL ANALYSIS

by

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In order to provide an accurate thermal analysis method of fiber-reinforced composites, a novel model based on a probabilistic representative volume element (RVE) is presented in this paper. Monte Carlo methods, probability analysis and finite element analysis have been applied together. The effective transverse thermal conductivity, heat flux field, and thermal gradient field of typical fiber-reinforced composites are examined. The criteria of RVE have been determined, and the minimal size for thermal analysis is obtained using the main statistics and the cross-entropy theory. At the same time, the fiber-to-matrix ratio of thermal conductivity and volume fraction have been changed to determine the influence on heat transfer inside fiber-reinforced composites. It is shown that different purposes of simulations lead to different minimal RVE sizes. The numerical results indicate that the non-dimensional minimal RVE sizes for calculating the effective thermal conductivity, heat flux, and thermal gradient are 30, 80, and 80, respectively. Compared with the volume fraction, the fiber-to-matrix ratio of the thermal conductivity has a more significant effect on minimal RVE size. When the thermal conductivity ratio increases, the minimal size of the RVE increases at first, then it remains almost unchanged.

Key words: *fiber reinforced composites, representative volume element, thermal analysis, minimal size*

Introduction

Fiber-reinforced composites (FRC) have been widely used in various industrial fields because of their low density, good thermal resistance and excellent structural properties. In many applications, it is desirable for the fatigue, fracture or lifetime of the FRC to be estimated, and this is especially the case when the materials are operating with thermal-mechanism loads. The thermal and mechanical responses of FRC materials are the keys of estimation, thus the relationship between the microstructure and macro properties like thermal conductivity and elastic modulus should be established first. However, the inhomogeneity and anisotropy of FRC microstructures leads to a complex physical procedure [1-3]. Many researchers voice concern

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over how to describe the microstructure in FRC materials, and also how to simulate physical procedures such as heat transfer or mechanics inside the materials.

Compared with the traditional equivalent inclusion treatment [4], the self-consistent method [5] and the thermoelectric analogy model [6], the representative volume element (RVE) model is more popular due to its broad applicability and reasonable accuracy, which was firstly studied by Hill [7]. The key using this method is to choose a valid RVE. Initially, a simple way to apply the RVE model is by assuming fibers within an FRC satisfy a periodicity hypothesis. Then the RVE with a typical periodic element can be used to predict the thermal or mechanical behavior as shown in the literature [8-10]. However, this simple RVE does not reflect the real microstructure of the FRC because of the use of the periodicity hypothesis. In fact, in real materials, fibers are usually distributed randomly, and this will affect the heat transfer or mechanics within FRC materials. Thus this randomness should be considered in the establishment of a valid RVE, as shown in the study of Buryachenko *et al.* [11], Trias [12], and Ganapathy *et al.* [13].

According to the concept of an RVE with randomly distributed fibers, a key problem in the simulation is how to determine the size of the RVE, which can guarantee the representation of the RVE and simultaneously reduce the cost of calculation. There have been some studies on the criteria of RVE size in different fields. Swaminathan *et al.* [14] investigated the size of a statistically equivalent volume element for a unidirectional composite. They pointed out that 50 fibers should be used in an RVE to determine the elastic properties correctly. The minimum size RVE when quantifying effective material properties of those exhibiting random patterns has also been noted by Rakow and Waas [15]. Their study shows that a region larger than 18 times the characteristic cell diameter is necessary when estimating the shear modulus of aluminum foam. Heinrich *et al.* [16] also studied the influence of RVE size on the computational accuracy of mechanical analysis on continuous fiber toughening composites. The result showed that at least 25 fibers should be used in the RVE for computation. In these studies, all the researchers focused on the effective thermal or mechanical properties and set them as the criteria of RVE size. These parameters are homogenized physical parameters, which are definitely important in engineering applications. However, according to the mentioned studies, the internal fields of heat flux or stress were totally heterogeneous. These heterogeneities were not fully considered if only the effective parameters were set as the criteria, which means that the RVE depending on these criteria can't reproduce the heat flux or stress maps accurately.

To improve the accuracy of an RVE, some researchers applied more parameters as criteria, including information on the internal physical field of an RVE. Trisa *et al.* [17] gave a detailed statistical analysis of the RVE size for a typical carbon fiber reinforced polymer. In their work, not only the effective mechanical properties (elastic modulus), but also the mean value and standard deviation of stress and strain fields were used as the criteria. The results showed that the minimal RVE size based on effective elastic modulus was 30 times the fiber radius, while the size based on the strain and stress field became 50 times, which was finally set as the minimum RVE size for a valid RVE. A quantitative definition of RVE size was also proposed in the work of Kanit *et al.* [18]. They pointed out that the RVE size depends on the investigated morphology or physical property, and the criteria in thermal studies are different from those in mechanical studies. Although there are some studies taking into account the characteristics of stress and strain when establishing the RVE for mechanical analysis, few works have been carried out for thermal analysis. Meanwhile, in the study of Trisa *et al.* [17], only the mean value and standard deviation of physical fields were compared. Actually, when considering the randomly distributed fibers, even the mean value of a physical field does not remain consistent, which may also follow a specific distribution. Therefore, when determining minimum RVE size, the relationship among these distributions gotten with different RVE sizes should be analyzed.

Recently, a math tool named cross-entropy, which can quantify the discrimination information between two distributions systematically, has been applied in many fields. In probability theory, entropy is a very important tool for measuring uncertain information. When Zadeh [19] first presented entropy to measure fuzziness by probability methods, he defined the basic notions (such as the mean and variance) in a more general way that relates them both as a fuzzy event and a probability measure. Mao *et al.* [20] extended the cross-entropy and entropy models to a general version, they also gave applications of pattern recognition and decision making to demonstrate the efficiency of the cross-entropy and entropy models. Qin [21] discussed the cross-entropy minimization model for a portfolio selection problem in a fuzzy environment, which minimizes the divergence of the fuzzy investment return from a priori one. Wang [22] applied the cross-entropy theory to power system reliability evaluations; considering the intermittency and fluctuation of a wind power system, different assessment criteria could be judged in a general way with the cross-entropy. All these studies show that the cross-entropy method has promising accuracy and advantages for analyzing the related information among random physical fields.

The present work is to obtain the multi-criteria for RVE by the cross-entropy method in the thermal analysis of long fiber-reinforced composites materials. The randomness of fibers' distribution was considered with a Monte Carlo simulation. The effective thermal conductivity (ETC), the heat flux field, and the thermal gradient field of a typical FRC were simulated. The cross-entropy method was applied to examine the relationship of a physical field's distribution. The criteria determining the validity of micro-models were chosen and analyzed according to these calculations. Then the influence of the volume fraction and the fiber-to-matrix ratio of thermal conductivity on minimal RVE size were also investigated.

Problem description

In general, the thermal properties of fibers along the longitudinal fiber direction are not necessarily the same as those in the transverse fiber direction. A typical RVE of an FRC is presented in fig. 1, which is usually established based on topological information on the FRC's cross-section. The circles represent fibers, while the other parts are matrix. In this paper, the size of the RVE is described by the dimensionless variable δ as shown in eq. (1):

$$\delta = \frac{L}{R} \tag{1}$$

where L is the side length of the RVE and R is the radius of the fiber. According to our test of a typical fiber reinforced composite by SEM; which was formed from T300 carbon fibers with an epoxy-resin matrix, the radius R is set as 2.5 μm in this manuscript. The non-dimensional size of δ (L/R) changes from 8 to 100. The purpose of this paper is to determine the minimal δ for a valid RVE in thermal analysis.

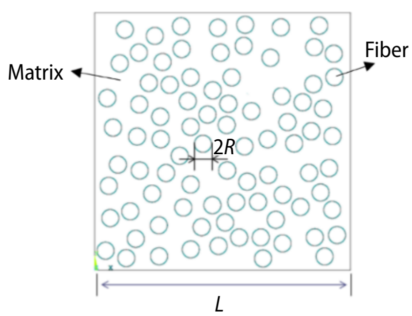


Figure 1. Schematic diagram of RVE size

The material in the present analysis is a long carbon fiber reinforced polymer (CFRP), whose main properties are set to the following values [23]: the transverse thermal conductivity of the T300 carbon fiber λ_F was 6.5 W/mK and the thermal conductivity of the epoxy resin matrix λ_M was 0.2 W/mK, leading to a thermal conductivity ratio of fiber to matrix r_c of 32.5. The number of fibers n is determined by the volume fraction of fibers V_f. The V_f is defined as the ratio of the fibers' area S_{fibers} to the RVE's area S_{RVE}, as shown in eq. (2):

$$V_f = \frac{S_{\text{fibers}}}{S_{\text{RVE}}} = \frac{n\pi R^2}{L^2} \tag{2}$$

Numerical procedure

The numerical procedure is shown in fig. 2. Firstly, RVE with random distributed fibers was established, *i. e.* a square with given size L was generated including some circles whose radius is R. This configuration stands for the RVE of composite, where these circles means the reinforced fibers. The positions of each fiber are given by the random sequential absorption algorithm. Then this configuration was meshed with triangular elements, using the ANSYS APDL's free meshing method. Finite element method was applied to solve the energy equation. Finally, the characteristics of temperature field and the effective thermal conductivity (ETC) can be obtained.

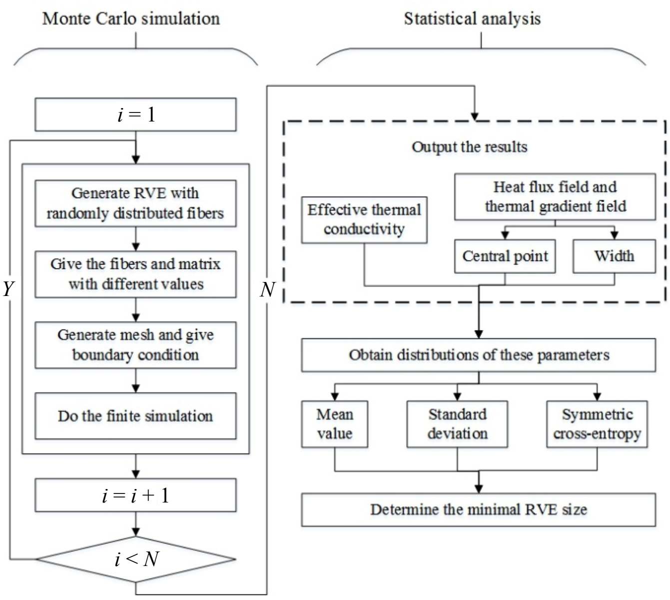


Figure 2. Numerical procedure

To get the effects of random fibers' distribution on ETC, Monte Carlo simulations have been applied. The RVE with those random fibers have been generated for N times in this paper, and the procedure above has been repeated for N times. In consequence, the distributions of ETC, expected point and width of the heat flux and thermal gradient fields have been obtained by statistical analyses.

Each technological process will be discussed in detail.

Random generation of fiber positions

The positions of each fiber in every RVE are random. The random sequential absorption algorithm [24] was used to generate the position of the fibers in each model. The position of each fiber in each RVE was random with a uniform distribution. This means that each point in the model has the same probability to contain a fiber.

In the generation, the following hypotheses are considered.

– There are no cracks in the models. Instead, they are completely continuous.

– The sections of fibers are circular, which means that no fiber is cut by the edge of an RVE.
– The co-ordinates of the center points of fibers are generated with the same statistical functions, and fibers will not overlap each other.

Mesh, boundary conditions and Monte Carlo simulation

The embedded cell approach that is applied in the model is shown in fig. 3. The circles represent fibers, while the other parts are matrix. Each model is meshed with triangular elements, using the ANSYS APDL's free meshing method. The boundary conditions can also be found in fig. 3. The constant heat flux boundary condition q = 400 kW/m^2 is applied on the left side of the model, while the boundary condition of the right side is q = –400 kW/m^2. The top and bottom sides are adiabatic.

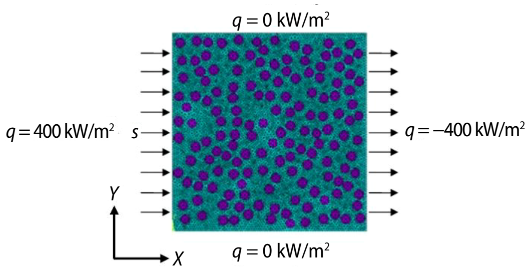


Figure 3. Computational domain and mesh

We apply the classical finite element method to obtain the temperature field, and get the corresponding ETC by the traditional Fourier equation. The detail is listed in eq. (3), where q is the heat flux, $\partial T/\partial x$ is the temperature gradient and λ_E represents ETC.

$$q = -\lambda_E \frac{\partial T}{\partial x} \tag{3}$$

It is worthwhile to point out that the ETC mentioned here only represents the thermal conductivity in the in-plane transverse direction, because the ETC along the longitudinal fiber direction can be easily and precisely calculated using the principle of equivalent inclusion with volume fraction.

The computational domain is required to have enough mesh to allow the simulation of the heat transfer without any mesh size correction. Therefore the model with δ = 40 is chosen to carry out the grid-independent test. The geometry of the micro-structure remains unchanged, but different mesh strategies are used. The non-dimensional mesh size (the ratio of minimum mesh length to R) changes from 0.1 to 1. The results in fig. 4 show that the variation of effective thermal conductivity λ_E is smaller than 1% with decreasing mesh size when less than 0.5. Therefore 0.5 is chosen to be the final mesh size in this study.

To get the distributions of the effective thermal conductivity, the expected point and the width of heat flux and thermal gradient fields, Monte Carlo simulations were carried out. The Monte Carlo method needs lots of multi-duplicated samples in order to obtain the probability statistics of events, so the chosen samples' number N is another important parameter in the simulation. Finally, the number of samples in this study was set as 1,000, depending on that the variation of $\mu(\lambda_E)$ and $\sigma(\lambda_E)$ should be smaller than 1%.

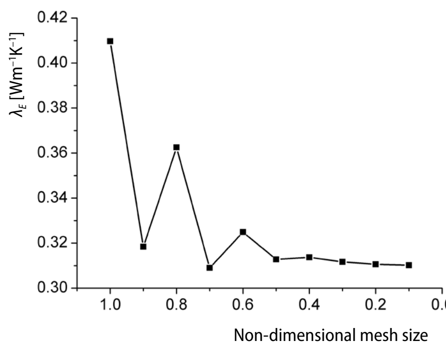


Figure 4. Evolution of λ_E with mesh size decreasing

Definitions of criteria for RVE size in the statistical thermal analysis

In the thermal analysis of an FRC in this paper, not only the effective thermal conductivity, but also the heat flux and thermal gradient field are considered and set as the criteria. The averaged equivalent heat transfer can be represented by the effective thermal conductivity, while the fluctuations of the temperature field can be revealed by the heat flux and thermal gradient.

Effective thermal conductivity

According to the Monte Carlo simulation used in this paper, the calculation of the temperature field is repeated many times, and the effective thermal conductivity λ_E is generated each time. So λ_E is a random variable that is normally distributed, which can be characterized by some statistics, such as the mean value and standard deviation. In this paper, the symmetric cross-entropy defined by Mao [20] is introduced to judge the discrimination between two normal distributions.

Let A be the reference object, and let A and B obey the normal distributions $\xi_a \sim N(\mu_a, \sigma_a^2)$ and $\xi_b \sim N(\mu_b, \sigma_b^2)$, respectively. Then the cross-entropy of A from B is:

$$CE(A,B) = \mu_a \ln\frac{2\mu_a}{\mu_a + \mu_b} + \sigma_a \ln\frac{2\sigma_a}{\sigma_a + \sigma_b} \tag{4}$$

Obviously, $CE(A,B)$ is not symmetric with respect to its arguments, so based on this concept, the symmetric cross-entropy is given by $DE(A,B) = CE(A,B) + CE(B,A)$. Moreover, $DE(A,B) = 0$ only if $a = b$.

The symmetric cross-entropy includes the message of both certainty and uncertainty, which can describe the discrimination between two normal distributions more systematically, compared with the relative variation of a single mean value or standard deviation, that is, $\mu(\lambda_E)$ and $\sigma(\lambda_E)$. So the distance between two distributions (A and B) of λ_E with different δ can be quantified by the symmetric cross-entropy:

$$DE(\lambda_E) = \mu(\lambda_E)_a \ln\frac{2\mu(\lambda_E)_a}{\mu(\lambda_E)_a + \mu(\lambda_E)_b} + \sigma(\lambda_E)_a \ln\frac{2\sigma(\lambda_E)_a}{\sigma(\lambda_E)_a + \sigma(\lambda_E)_b} \tag{5}$$

Heat flux field

According to the work of Trisa *et al.* [25], the internal physical field can be described by the mean value and standard deviation. Similar parameters are introduced in this paper to describe the heat flux field, which are defined as the expected point μ_{TF} and width σ_{TF}:

$$\mu_{TF} = \frac{1}{N}\sum_{i}^{N} q_i \tag{6}$$

$$\sigma_{TF} = \sqrt{\frac{1}{N}\sum_{i=1}^{N} (q_i - \mu_{TF})^2} \tag{7}$$

where q_i is the heat flux through each grid node, and N is the number of samples in the Monte Carlo simulation. The μ_{TF} and σ_{TF} are random variables that are normally distributed according to the Monte Carlo simulation. So both of them can be characterized by a mean value and standard deviation, that is, $\mu(\mu_{TF}), \sigma(\mu_{TF}), \mu(\sigma_{TF}), \sigma(\sigma_{TF})$. Similarly, the distance between two distributions of μ_{TF} or σ_{TF}, which relate to two different sizes, can be quantified by the symmetric cross-entropy:

$$DE(\mu_{TF}) = \mu(\mu_{TF})_a \ln \frac{2\mu(\mu_{TF})_a}{\mu(\mu_{TF})_a + \mu(\mu_{TF})_b} + \sigma(\mu_{TF})_a \ln \frac{2\sigma(\mu_{TF})_a}{\sigma(\mu_{TF})_a + \sigma(\mu_{TF})_b} \tag{8}$$

$$DE(\sigma_{TF}) = \mu(\sigma_{TF})_a \ln \frac{2\mu(\sigma_{TF})_a}{\mu(\sigma_{TF})_a + \mu(\sigma_{TF})_b} + \sigma(\mu_{TF})_a \ln \frac{2\sigma(\sigma_{TF})_a}{\sigma(\sigma_{TF})_a + \sigma(\sigma_{TF})_b} \tag{9}$$

It is worthwhile to point out that the expected point μ_{TF} and width σ_{TF} also represent the mean value and standard deviation of the heat flux field. To distinguish these parameters from the mean value and standard deviation of themselves, *i. e.* $\mu(\mu_{TF})$, $\sigma(\mu_{TF})$, $\mu(\sigma_{TF})$, $\sigma(\sigma_{TF})$, the μ_{TF} and σ_{TF} are named as expected point and width specifically, and the symmetric cross-entropies are calculated with non-dimensional method.

Thermal gradient field

Similar to the heat flux field, the thermal gradient field also can be described by the expected point μ_{TG} and width σ_{TG}, and the criteria are $\mu(\mu_{TG})$, $\sigma(\mu_{TG})$, $\mathrm{DE}(\mu_{TG})$, $\mu(\sigma_{TG})$, $\sigma(\sigma_{TG})$, $\mathrm{DE}(\sigma_{TG})$, whose method of calculation are same with the corresponding parameters in the heat flux field.

Consequently, the variables that are considered as criteria for the determination of the minimal RVE size in this paper are the main statistics (including mean value, standard deviation and symmetric cross-entropy) of effective thermal conductivity, heat flux and thermal gradient fields, as shown in tab. 1. Each of them is satisfied by an RVE size δ. The criterion that is satisfied for a larger δ will determine the required minimal size for a valid RVE.

Table 1. Summary of analyzed criteria

Study object	Mean value	Standard deviation	Symmetric cross-entropy
Effective thermal conductivity, [Wm^{-1}K^{-1}]	$\mu(\lambda_E)$	$\sigma(\lambda_E)$	$DE(\lambda_E)$
Expected point of heat flux field, [kWm^{-2}]	$\mu(\mu_{TF})$	$\sigma(\mu_{TF})$	$DE(\mu_{TF})$
Width of heat flux field, [kWm^{-2}]	$\mu(\sigma_{TF})$	$\sigma(\sigma_{TF})$	$DE(\sigma_{TF})$
Expected point of thermal gradient field, [Km^{-1}]	$\mu(\mu_{TG})$	$\sigma(\mu_{TG})$	$DE(\mu_{TG})$
Width of thermal gradient field, [Km^{-1}]	$\mu(\sigma_{TG})$	$\sigma(\sigma_{TG})$	$DE(\sigma_{TG})$

In this paper, the criteria of relative variation of μ and σ are taken as 5%. Simultaneously, for the symmetric cross-entropy, the criteria are set at 0.005.

Operating conditions

To get the influence of various properties of FRC such as the thermal conductivity ratio of fiber to matrix, r_c, the volume fraction, V_f, on the minimum size of RVE, these two parameters were changed in simulations. Details are listed in tab. 2.

Table 2. Calculation cases

Variables	Value
Thermal conductivity ratio, r_c	2, 10, 32.5, 65, 130
Volume fraction, V_f,	0.1, 0.2, 0.3, 0.4

Results and discussions

Temperature field and heat flux field

The contours of temperature and heat flux inside two samples of RVE are shown in fig. 5. The RVE sizes of these two samples are 40, and the volume fraction is 0.3 for all the results in this section, while the fibers are scattered randomly.

Figure 5 shows that the isothermals are not straight lines, and that instead they present a wave shape. This indicates that the heat transfer inside a heterogeneous FRC isn't uniform. This can be further demonstrated with the distribution of heat flux in fig. 5(b). Higher local heat flux is observed at the region inside and very close to fibers due to the greater thermal conductivity of fiber. More heat will be transferred when these fibers gather together. The path of heat transfer is therefore dependent upon the distribution of fibers, and this is obviously due to the difference in thermal conductivity between the fibers and the matrix.

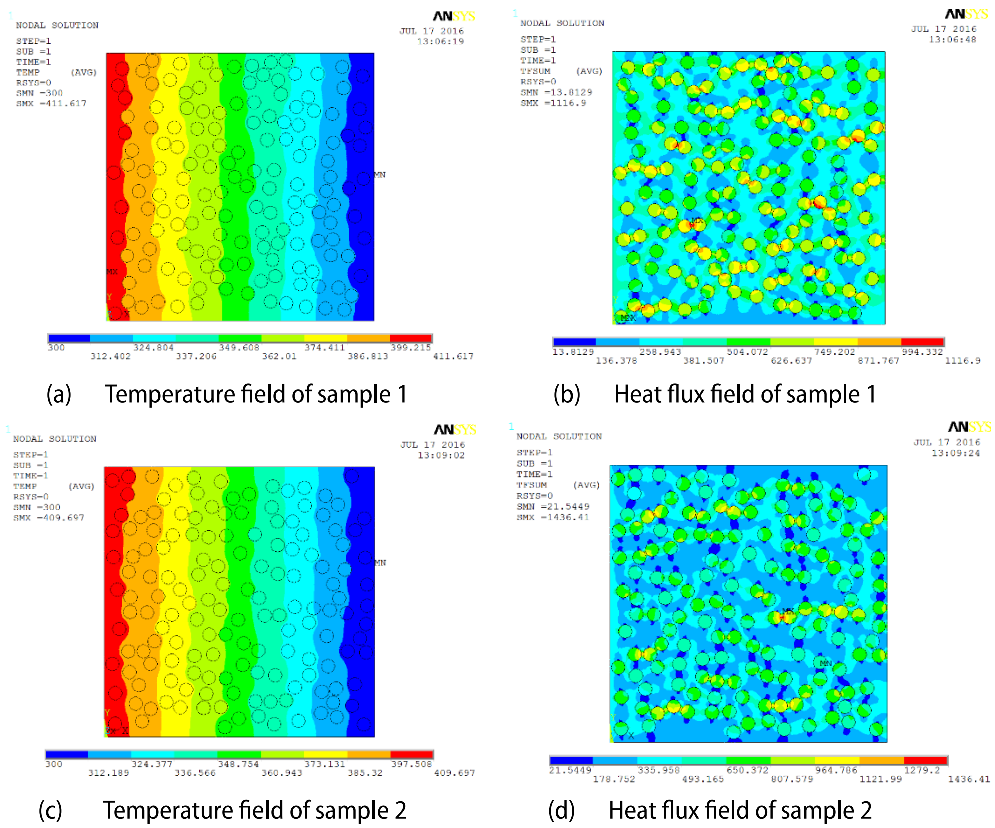


Figure 5. Temperature field and heat flux field of FRC

At the same time, the isothermal lines are not the same in the two samples shown in figs. 5(a) and 5(c). Similar phenomena are seen in the heat flux field, as shown in figs. 5(b) and 5(d). This can be attributed to the random position of fibers.

In these two samples, the volume fraction and the total heat flux through boundaries are all consistent, as we see in calculations. The average values of temperature (354.03 K for sample 1, 353.57 K for sample 2) are also almost the same according to the results. There are obvious fluctuations in local temperature and heat flux, including the location of the isotherm, the high temperature area and the maximum heat flux. For example, the maximum heat flux of sample 1 is $1.1169 \cdot 10^3$ kW/m^2, while the maximum heat flux of sample 2 is $1.4364 \cdot 10^3$ kW/m^2, giving a relative error of 29%. In consequence, to get the fluctuations and the correlations, the traditional numerical simulation with RVE is not suitable, and the probabilistic analysis is a promising method.

Effective thermal conductivity

The evolution of $\mu(\lambda_E)$ and $\sigma(\lambda_E)$ with increasing RVE size are shown in figs. 6(a) and 6(b). The results show that small relative variations of $\mu(\lambda_E)$ and $\sigma(\lambda_E)$ that are lower than 5% are obtained from $\delta = 18$ and $\delta = 30$, respectively. The relative variations are however much less than 5% when $\delta = 100$. This means that the RVE model with $\delta = 100$ has the same statistics over the whole material. Therefore, the model with $\delta = 100$ can be regarded as a reference in the calculation of $DE(\lambda_E)$.

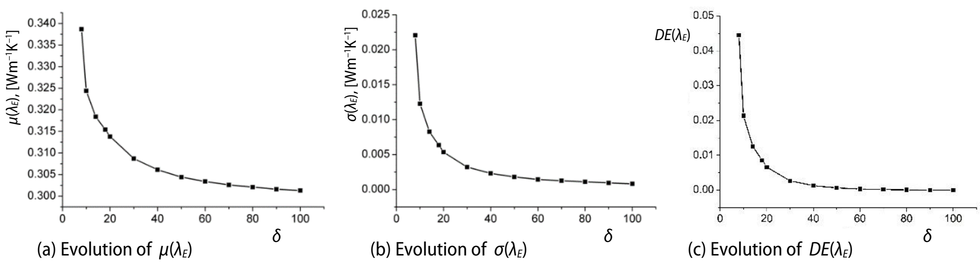


Figure 6. Evolution of the $\mu(\lambda_E)$, $\sigma(\lambda_E)$ and $DE(\lambda_E)$ of effective thermal conductivity

Figure 6(c) shows the evolution of $DE(\lambda_E)$ between each size and $\delta = 100$. It can be seen that $DE(\lambda_E)$ is smaller than 0.005 from $\delta = 30$. Therefore $\delta = 30$ can be regarded as the minimal RVE size when the effective thermal conductivity is the noteworthy parameter.

Heat flux field

Heat flux field, the heat flux field can be described by μ_{TF} and σ_{TF}. The μ_{TF} represents the expected point of the heat flux field, and σ_{TF} represents the width of the heat flux field.

Convergence of the μ_{TF}

Figsures 7(a) and 7(b) give the rules of $\mu(\mu_{TF})$ and $\sigma(\mu_{TF})$ with varying RVE size. The results show that the relative variation of $\mu(\mu_{TF})$ and $\sigma(\mu_{TF})$ are lower than the 5% convergence standard with $\delta = 70$ and $\delta = 40$, respectively.

The $\mu(\mu_{TF})$ is found to be 760.52 kW/m^2 when $\delta = 90$, and it changes to 766.84 kW/m^2 when $\delta = 100$, giving a relative variation of about 0.83%, which is much less than 5%. Therefore, the model with $\delta = 100$ can be the reference object in the calculations of $DE(\mu_{TF})$. Figure 7(c) shows the result of symmetric cross-entropy analysis. According to the result, $DE(\mu_{TF})$ is below 0.005 if δ is larger than 40.

Additionally, the RVE sizes based on the λ_E and μ_{TF} are 30 and 70, respectively. The $\mu(\mu_{TF})$ is 656.04 kW/m^2 and 737.36 kW/m^2 when δ equals 30 and 70, for a relative variance of 11%. It means that the RVE generated only depended on the ETC will lead to a relative error of 11% in the simulation of the mean value of the heat flux field.

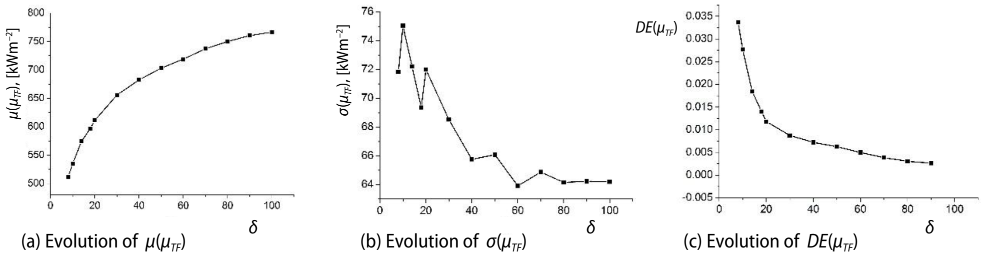


Figure 7. The $\mu(\mu_{TF})$, $\sigma(\mu_{TF})$ and $DE(\mu_{TF})$ of the expected point in heat flux field

Convergence of the σ_{TF}

The evolution of $\mu(\sigma_{TF})$ and $\sigma(\sigma_{TF})$ with increasing RVE size is shown in figs. 8(a) and 8(b). In the results, relative variations smaller than 5% of the $\mu(\sigma_{TF})$ and $\sigma(\sigma_{TF})$ are obtained from δ = 70 and δ = 40, respectively. The relative variations are far less than 5% when δ = 100, and therefore the model with δ = 100 can also be the reference for calculations of $DE(\sigma_{TF})$. Figure 8(c) shows the evolution of $DE(\sigma_{TF})$. It is found to start at values lower than 0.005 at δ = 40.

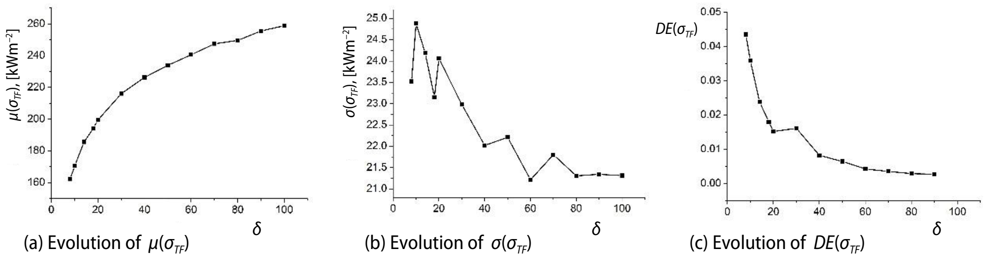


Figure 8. The $\mu(\sigma_{TF})$, $\sigma(\sigma_{TF})$ and $DE(\sigma_{TF})$ of the width of heat flux field

Considering all the results (δ = 70 for $\mu(\mu_{TF})$, δ = 40 for $\sigma(\mu_{TF})$, δ = 40 for $DE(\mu_{TF})$, δ = 70 for $\mu(\sigma_{TF})$, δ = 40 for $\sigma(\sigma_{TF})$, δ = 40 for $DE(\sigma_{TF})$), the minimal RVE size is found to be 70 when the heat flux field is the object of concern.

Convergence of the thermal gradient field

In fig. 9, the curves of $\mu(\mu_{TG})$, $\sigma(\mu_{TG})$, and $DE(\mu_{TG})$ have been plotted. The results show that small relative variations, lower than 5% of $\mu(\mu_{TG})$ and $\sigma(\mu_{TG})$, are obtained for δ = 80 and δ = 50. The $DE(\mu_{TG})$ between models with δ = 40 and δ = 100 is less than 0.005.

The evolution of $\mu(\sigma_{TG})$ and $\sigma(\sigma_{TG})$ is shown in fig. 10. The results show that small relative variations, lower than 5% of the $\mu(\sigma_{TG})$ and $\sigma(\sigma_{TG})$, are obtained from δ = 60 and δ = 40. At the same time, the $DE(\sigma_{TG})$ begins lower than 0.005 from δ = 50.

Comparing the results the RVE sizes based on λ_E and μ_{TG} are 30 and 80, respectively. The relative variance of $\mu\left(\mu_{TG}\right)$ is 14%, which means that the RVE generated, depending on the ETC only, will lead to a relative error of 14% in the simulation of mean value of the thermal gradient field. In engineering applications, this relative error will furthermore decrease the accuracy in the thermal stress analysis and the life estimation.

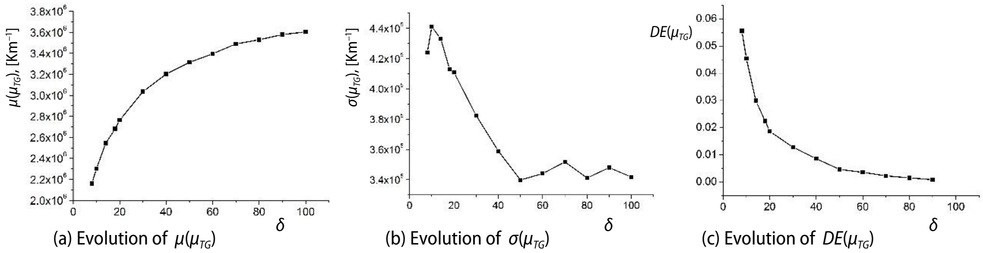


Figure 9. The $\mu(\mu_{TG})$, $\sigma(\mu_{TG})$ and $DE(\mu_{TG})$ of the expected point in the thermal gradient field

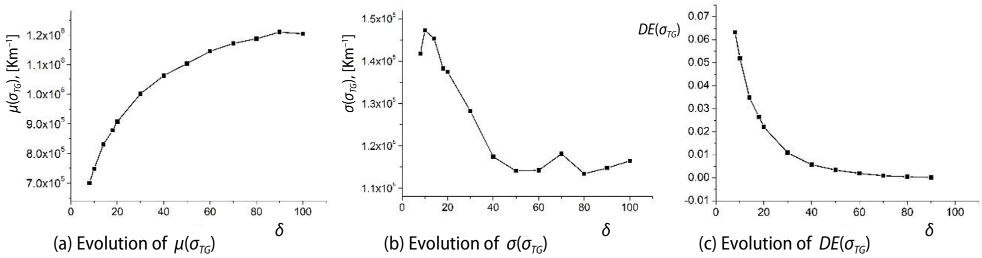


Figure 10. The $\mu(\sigma_{TG})$, $\sigma(\sigma_{TG})$ and $DE(\sigma_{TG})$ of the width in the thermal gradient field

Table 3 summarizes the results obtained for each criterion. According to the final result, for the long fiber-reinforced composite studied in this paper, the minimal size of an RVE in thermal analysis is $\delta = 80$.

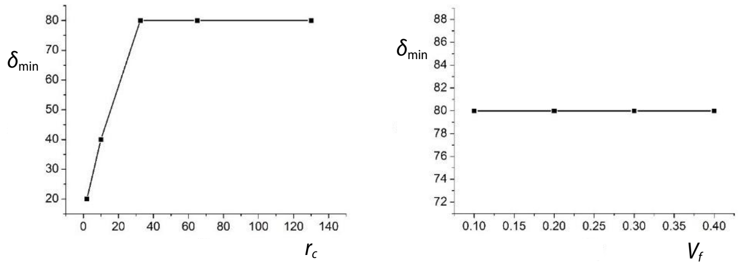
Table 3. Summary of analyzed criteria and results

Study object	Criteria	Result
Effective thermal conductivity	Mean value	$\delta \geq 18$
	Standard deviation	$\delta \geq 30$
	Symmetric cross-entropy	$\delta \geq 30$
Expected point of heat flux field	Mean value	$\delta \geq 70$
	Standard deviation	$\delta \geq 40$
	Symmetric cross-entropy	$\delta \geq 40$
Width of heat flux field	Mean value	$\delta \geq 70$
	Standard deviation	$\delta \geq 40$
	Symmetric cross-entropy	$\delta \geq 40$
Expected point of thermal gradient field	Mean value	$\delta \geq 80$
	Standard deviation	$\delta \geq 50$
	Symmetric cross-entropy	$\delta \geq 40$
Width of thermal gradient field	Mean value	$\delta \geq 60$
	Standard deviation	$\delta \geq 40$
	Symmetric cross-entropy	$\delta \geq 50$

Influences of the r_c and V_f on minimal RVE size

Repeating the analysis procedures presented in part *Results and discussion* when different r_c and V_f are considered, the final minimal sizes of RVE are shown in fig. 11.

It can be found that the minimal RVE size gets larger with higher r_c (from 2 to 32.5). It tends to be consistent when r_c continues to increase (from 32.5 to 130). This is because a larger temperature difference would be generated with higher r_c (from 2 to 32.5), which means that the RVE must be large enough to eliminate the non-uniformity in heat transfer. But if the r_c is too high, the heat transfer inside the FRC is determined mainly by fibers. The fluctuations of the results with different representative volume sizes are covered, therefore the minimal RVE size is shown to be consistent when the r_c is larger than 32.5.



(a) Minimal RVE size with increasing r_c (b) Minimal RVE size with increasing V_f

Figure 11. Minimal RVE size affected by r_c and V_f

The results also show that the final minimal RVE sizes for thermal analysis under different volume fraction conditions are always 80. This result is direct evidence that the volume fraction has little influence on the RVE's minimal size.

Conclusions

A novel model based on the probabilistic representative volume element (RVE) is presented in this paper. A variety of criteria to determine the minimal RVE size in thermal analysis of fiber-reinforced composites (FRC) are applied and discussed. The criteria are the mean value, the standard deviation and the symmetric cross-entropy of the effective thermal conductivity, the heat flux field and the thermal gradient field. The influence of the thermal conductivity ratio (fibers to matrix) and volume fraction upon the minimal RVE size are also studied.

All of the numerical results show that:

- the symmetric cross-entropy has a good ability to quantify the discrimination messages between different distributions of a physical field, which is essential for the determination of minimal RVE size,
- different purposes of simulation will result in different minimal RVE sizes. In this paper, the required RVE sizes of effective thermal conductivity, heat flux field and thermal gradient field are 30, 70 and 80, respectively, so the minimal size of the RVE is 80,
- the RVE only depended on the effective thermal conductivity, which will lead to errors in the simulation of heat flux and thermal gradient fields, further decreasing the accuracy in the thermal stress analysis and the life estimation of the FRC,
- the thermal conductivity ratio of fibers to matrix has distinguished the influence on the minimal size of the RVE. The larger minimal RVE size is found to have a higher thermal conductivity ratio (from 2 to 32.5), while it tends to be saturated if the thermal conductivity ratio has high values (from 32.5 to 130), and
- the volume fraction has little influence on the determination of minimal RVE size.

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Nomenclature

L – side length of RVE and R is the radius of the fiber, [μm]
q – heat flux, [kWm^{-2}]
R – radius of fiber, [μm]

r_c – thermal conductivity ratio of fiber to matrix, [–]
V_f – volume fraction of fibers, [–]

Greek symbols

δ – dimensionless size of RVE, [–]
λ_E – effective thermal conductivity, [Wm^{-1}K^{-1}]
λ_F – thermal conductivity of fibers, [Wm^{-1}K^{-1}]
λ_M – thermal conductivity of matrix, [Wm^{-1}K^{-1}]
μ – mean value, [–]
σ – standard deviation, [–]

Subscripts

TF – heat flux field
TG – thermal gradient field

References

[1] Rabearison, N., *et al*., A FEM Coupling Model for Properties Prediction during the Curing of an Epoxy Matrix, *Comput. Mater. Sci., 45* (2009), 3, pp. 715-724
[2] Corden, T. J., *et al*., The Mechanisms of Interlaminar Cracking in Thick Resin Transfer Moulded Composite Cylinders, *Compos. A. Appl. Sci. Manuf., 29* (1998), 4, pp. 455-464
[3] Plepys, A., Farris, R., Evolution of Residual Stresses in Three-Dimensionally Constrained Epoxy Resins, *Polymer, 31* (1990), 10, pp. 1932-1936
[4] Rayleigh, L., LVI on the Influence of Obstacles Arranged in Rectangular Order upon the Properties of a Medium, *The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science, 34* (1892), 211, pp. 481-502
[5] Hasselman, D. P., Johnson, L. F., Effective Thermal Conductivity of Composites with Interfacial Thermal Barrier Resistance, *Journal of Composite Materials, 21* (1987), 6, pp. 508-515
[6] Zou, M., *et al*., Study on Optimization of Transverse Thermal Conductivities of Unidirectional Composites, *Journal of heat transfer, 125* (2003), 6, pp. 980-987
[7] Hill, R., Elastic Properties of Reinforced Solids: Some Theoretical Principles, *J. Mech Phys. Solid, 11* (1963), 5, pp. 357-372
[8] Islam, M. R., Pramila, A., Thermal Conductivity of Fiber Reinforced Composites by FEM, *Journal of Composite Materials*, *33* (1999), 18, pp. 1699-1715
[9] Klett, J. W., *et al*., Finite-Element Modeling of Heat Transfer in Carbon/Carbon Composites, *Composites Science and Technology, 59* (1999), 4, pp. 593-607
[10] Car, E., *et al*., Numerical Simulation of Fiber Reinforced Composite Materials: Two Procedures, *Inter. J. Solid Struct.*, *39* (2002), 39, pp. 1967-1986
[11] Buryachenko, V. A., *et al*., Quantitative Description and Numerical Simulation of Random Microstructure of Composites and Their Effective Elastic Moduli, *Int. J. Solids Struct.*, *40* (2003), 1, pp. 47-72
[12] Trias, D., Analysis and Simulation of Transverse Random Fracture of Long Fiber Reinforced Composite, Ph. D. Thesis, University of Girona, Catalonia, Spain, 2005
[13] Ganapathy, D., *et al*., An Effective Unit Cell Approach to Compute the Thermal Conductivity of Composites with Cylindrical Particles, *Journal of Heat Transfer, 127* (2005), 6, pp. 553-559
[14] Swaminathan, S., *et al*., Statistically Equivalent Representative Volume Elements for Unidirectional Microstructures: I without Damage, *J. Compos. Mater., 40* (2006), 7, pp. 583-604
[15] Rakow, J. F., Waas, A. M., Size Effects in Metal Foam Cores for Sandwich Structure, *AIAA J., 42* (2004), 7, 1331-7
[16] Heinrich, C., *et al*., The Influence of the Representative Volume Element (RVE) Size on the Homogenized Response of Cured Fiber Composites, *Modelling and Simulation in Materials Science and Engineering*, *20* (2012), 7, 075007
[17] Trias, D., *et al*., Determination of the Critical Size of a Statistical Representative Volume Element (SRVE) for Carbon Reinforced Polymers, *Acta Materialia, 54* (2006), 13, pp. 3471-3484
[18] Kanit, T., *et al*., Determination of the Size of the Representative Volume Element for Random Compistes: Statistical and Numerical Approach, *International Journal of Solids and Structures*, *40* (2003), 13-14, pp. 3647-3679
[19] Zadeh, L.A., Probability Measures of Fuzzy Events, *Journal of Mathematical Analysis and Applications, 23* (1968), 2, pp. 4212-427
[20] Mao, J. J., *et al*., A Novel Cross-Entropy and Entropy Measures of IFSS and Their Applications, *Knowledge – Based Systems, 48* (2013), 2, pp. 37-45
[21] Qin, Z. F., *et al*., Portfolio Selection Based on Fuzzy Cross-Entropy, *Journal of Computational and Applied Mathematics*, *228* (2009), 1, pp. 139-149

[22] Wang, Y., Power System Short-Term Reliability Evaluations Based on Cross-Entropy Theory, Ph. D. thesis, College of Electrical Engineering, Zhejiang University, Zhejiang, China, 2014
[23] He, F., *Carbon Fiber & Graphite Fiber*, Chemical Industry Press, Beijing, 2010
[24] Ohser, J., Mucklich, F., Statistical Analysis of Microstructures in Materials Science, *Statistics in Practice,* John Wiley and Sons, New York, USA, 2000
[25] Brockenborough, J. R., *et al*., Deformation of Metal-Matrix Composites with Continuous Fibers: Geometrical Effects of Fiber Distribution and Shape, *Acta Metall Mater*, *39* (1991), 5, pp. 735-752

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