NUMERICAL INVESTIGATION OF EFFECTIVE THERMO-MECHANICAL PROPERTIES IN SHORT FIBRE COMPOSITES

I. Ioannou*, A. Hodzic, I. Gitman

Composite Systems Innovation Centre, Department of Mechanical Engineering, The University of Sheffield, Sheffield, UK

**mep10ii@sheffield.ac.uk*

Keywords: RVE, homogenization, stochastic parameters, short fiber composites

Abstract

The following study aims to investigate the contribution of various micromechanical parameters on the macroscopic response of a two-phase short fiber composite using numerical methods. Parameters like fiber length and fiber orientation were extensively studied under the concept of Representative Volume Element (RVE) in order to quantify the contribution of those parameters on the macroscopic response of the material. Results show that the macroscopic response of a composite material is strongly influenced by thermo-physical changes in the microstructure. Mechanical and thermal responses are compared for various cases of fiber orientation, fiber aspect ratio and length distributions. A comparison between RVE response and analytical micromechanical models showed a good agreement.

1. Introduction

Short fiber composite materials are very attractive systems due to their relatively low-cost manufacturing processes, their enhanced thermo-mechanical properties and lightweight load-bearing capability. Due to those reasons SFRC are widely used in numerous applications with a clear aim to replace traditional engineering materials. Due to the growing use of SFRCs, engineers need to consider the environmental impact of this kind of materials and propose solutions to overcome this problem. The field of short fiber composites has been studied widely. A pioneering work was published in 1952 [1], presenting the shear lag model that was able to calculate the effective stiffness of a composite, and it also offered a solution about the normal and shear stress distribution in a fiber. Further, Eshelby's [3] work established a cornerstone in the field of micromechanics. Solutions from Eshelby's theory have been widely used in the mean field methods [4, 5]. The following work focuses on the thermo-mechanical properties of thermoplastic short fiber composites. Thermoplastic matrices are recycles materials with much less environmental impact compared with thermosets. It has been reported in the literature [6-8] that the performance of SFRCs strongly dependents on the micromechanical parameters and on the manufacturing processes. There are mainly two manufacturing processes used for producing short fiber composites: injection molding and extrusion compounding. Analysis of the influence of manufacturing processes is out of the focus of this research, however the secondary results of the manufacturing process such as random fiber length and random orientation of fibers have been considered in this study. Those parameters were distinctly simulated and conclusions about the influence of each micromechanical parameter were evaluated. More precisely, this study aims to characterize a two phase composite material consisting of glass fibers embedded in a thermoplastic matrix.

The properties varied in this investigation are longitudinal and transverse effective stiffness, effective shear stiffness, longitudinal and transverse thermal conductivity and longitudinal and transverse linear coefficients of thermal expansion. All the aforementioned mechanical, thermal and thermo-mechanical properties have been investigated for constant length of fibers, random distribution of fibers length, unidirectional aligned fibers, mis-aligned fibers and randomly oriented fibers. In the case of constant fibers length, effective properties were studied for three different aspect ratios.

2. Methodology

In order to investigate the effective mechanical, thermal and thermo-mechanical properties of short fiber reinforced thermoplastic material the concept of RVE was implemented. According to RVE concept simple virtual experiments were carried out for the evaluation of the effective properties. The process can be divided into four distinct steps. The first step involves the creation of microstructures, while the second step involves the implementation of boundary conditions and the response of the stress and strain field. The third steps applies an average homogenization approach to the existing stress and strain fields, while the last step involves a statistical analysis of the homogenized results in order to evaluate the quality of the derived effective properties.

Solutions for the stress and strain fields were obtained by implementing the numerical method of finite element analysis. The microstructure of the models were created in Matlab and transferred to the commercial finite element code Abaqus, through python scripting, for further analysis. The resulting stress and strain fields were subsequently re-introduced into Matlab for a post-processing homogenization process and a further statistical investigation of the derived effective properties.

2.1. Packing procedure

The major advantage in calculating effective properties using numerical methods against analytical approaches is the ability to accurately simulate the distribution of microstructure, and in general to include the information from the composite microstructure. This can be achieved by designing distinct fibers in a container-domain. This is not a trivial matter and is also known as *packing problem*. In the current study, in order to overcome the packing problem, an algorithm was designed to create multiple microstructures in two-dimensional environment. The characteristic flow chart of the basic algorithm is shown in Figure 1.

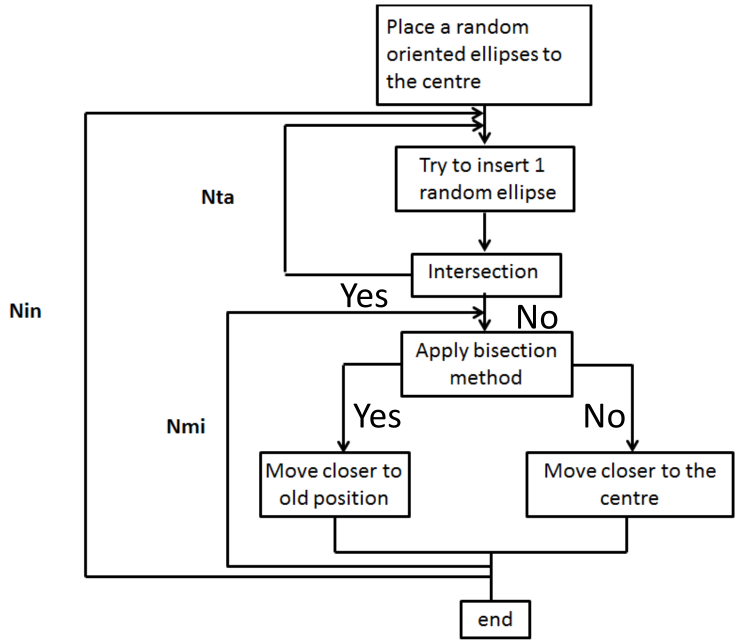

Figure 1 The flow chart of the developed algorithm.

As it can be seen in Fig. 1, the algorithm is using a basic loop in order to place fibers in a random position in space, which is repeated as many times as the number of fibers. A secondary control loop checks for intersection between fibers by calculating the distance of the perimeter while the last iterative loop implements a bisection method in order to gather fibers toward the center of the square element, in order to increase the maximum achievable volume fraction. Typical representation of the microstructure created by the aforementioned algorithm can be seen in Figure 2. Six representations in Fig. 2 show RVE for three different orientations, using constant fiber length distribution for three different aspect ratios.

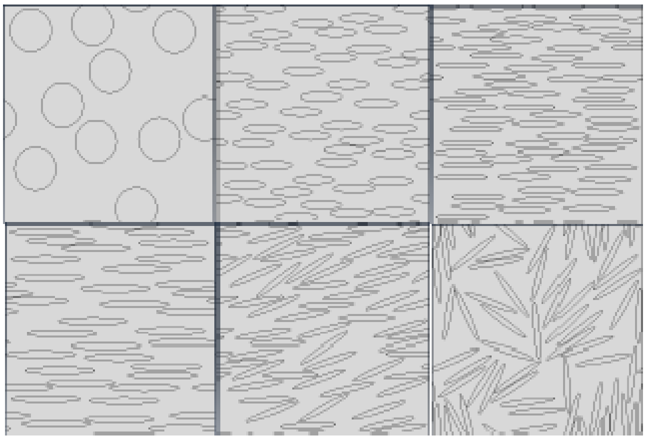

Figure 2 Representative microstructures for three different orientations and three different aspect ratios (AR).

2.2. Volume average homogenization approach

Homogenization can be interpreted as a general trend of the behavior of a material that is inhomogeneous on a lower length scale, however in terms of energetic equivalent, a homogeneous reference material on a higher length scale can be defined. The response of the material under a simple uniaxial force as either longitudinal or transverse tension was evaluated by measuring local values of the stress and strain field for each element, and then those values were implemented in an average homogenization model. Average stresses and average strains can be calculated by using equation (1) and (2). The aforementioned equations are stated the average stress and average strain theorem and involve the volume integration of local field values of stresses and strains. The resultant average stress and strains value can be used in (3) in order to calculate effective mechanical properties. In a similar way as the mechanical average field and the thermal average field of heat flux can be evaluated through an area summation (4), calculation of effective thermal conductivity is possible through (5):

$$\overline{\langle\sigma\rangle}_{ij} = \frac{1}{V}\int_V \sigma_{ij}(x)dV \tag{1}$$

$$\overline{\langle\varepsilon\rangle}_{ij} = \frac{1}{V}\int_V \varepsilon_{ij}(x)dV \tag{2}$$

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} \tag{3}$$

$$Q_i = \sum_{j=1}^{N} q_i^j A^j \tag{4}$$

$$k_i = q_i \frac{\Delta X}{\Delta T} \qquad (5)$$

2.3. Chi square statistical test

To address all possible combinations of the RVE cases under consideration (three different orientations, three different aspect ratios, three different RVE sizes and for random fiber's length distribution), five different realizations were created. With the term realization is meant that an RVE has the same volume fraction, the same orientation distribution, the same aspect ratio and the same RVE's size, however different distribution of fiber's position in space. Those five different realizations enable conclusions achieved through a statistical test for the representativeness of each size, and establish how this representativeness is affected by orientation or aspect ratio or the effective property under investigation. Chi square test is expressed in (6).

$$x^2 = \sum_{j=1}^{k} \frac{\left(Y_j - Y_{av}\right)^2}{Y_{av}} \qquad (6)$$

The test was applied for three statistical DoF and for 95% accuracy. A typical example of chi square values in respect with RVE's size for longitudinal, transverse and shear effective stiffness with both thermal conductivities for AR=1 can be seen in Figure 3.

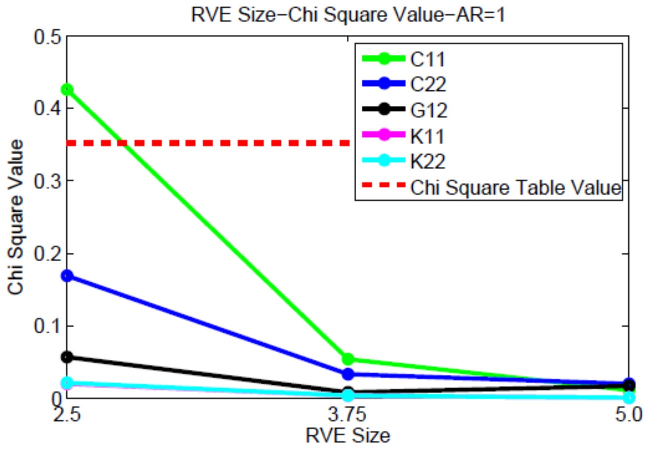

Figure 3 A typical example of chi square test distribution as a function of RVE size.

3. Numerical models

Numerical models were developed in the commercial finite element code Abaqus 6.10-2 once the microstructure was imported from Matlab through python scripting. All the RVEs designed for investigation of mechanical properties were meshed with CPS3 plain stress triangular elements. The choice of triangular elements distribution was one-way due to the difficulty of using *quad* elements in a very stochastic microstructure. A very basic convergence study took place for the first representative size and mesh density was higher for the fibers compared with the matrix. Due to the stochastic nature of the matrix structure elements were not always the same size and as a result for some cases few elements were distorted and exhibited an artificial higher local stiffness. For all the cases models with unacceptable number of distorted elements were rejected. A typical example of mesh with CPS3 triangular elements can be seen in Figure 4.

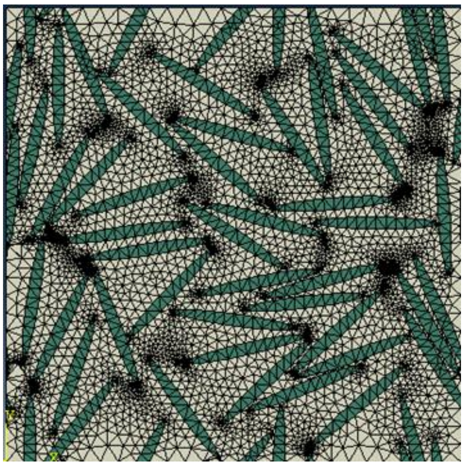

Figure 4 A typical example of RVE mesh with CPS3 elements.

Periodic boundary conditions were used as can be seen in (7). This type of boundary condition is widely used in the case of simulation of a small part of a structure in order to derive properties for the whole domain of the structure.

$$u_i^{j+} - u_i^{j-} = \bar{\varepsilon}_{kl}\left(x_k^{j+} - x_k^{j-}\right) = \bar{\varepsilon}_{kl}\Delta x_k^j \tag{7}$$

4. Result and Discussion

Results for the local stress and strain field were obtained after applying the boundary conditions and solving the constitutive equations for the RVE. Un-deformed and deformed shapes of the RVE showing the developed strain field for AR=1, AR=5, and AR=10 can be seen in Figure 5.

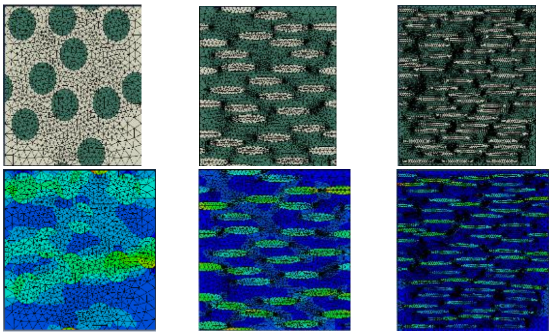

Figure 5 Deformed and un-deformed shapes of RVE for AR=1, 5 and 10.

A typical example of results for longitudinal effective stiffness, transverse effective stiffness and effective shear stiffness can be seen in Figure 6.

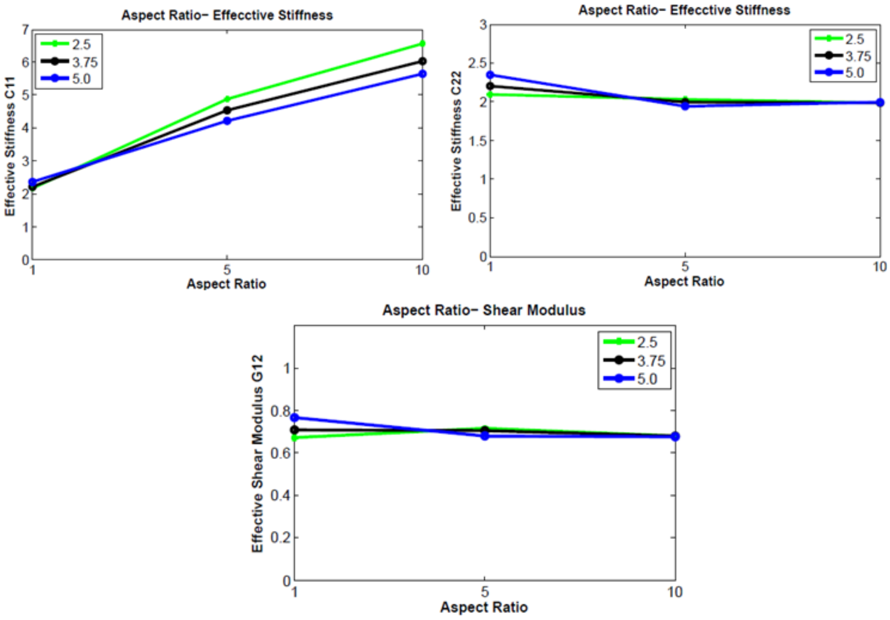

Figure 6 A typical example of effective properties as a function of AR for three different sizes.

The characterization of thermal and mechanical effective properties has been studied through numerical simulation. The developed models cover numerous combinations of microstructural parameters. Results show that micromechanical parameters such as aspect ratio and fiber orientation can strongly influence the macroscopic response of short fiber composites. In this study, evaluation of the representativeness of the RVE size was carried out through a statistical test. Results showed that the representative size can be expressed as a function that accounts for the volume fraction, the fiber length and the nature of the micromechanical parameters.

References

[1] H.L. Cox, The elasticity and strength of paper and other fibrous materials, *British journal of applied physics*,72-79,(1951).

[2] J.C. Halpin, The Halpin-Tsai equations: A review. *Polymer engineering and science*, **16**, 344-352,1976.

[3] J.D. Eshelby. The determination of the elastic field of an ellipsoidal inclusion, and related problems, proceedings of the royal society, London, UK, (1957).

[4] T. Mori and K. Tanaka, Average stress in matrix and average elastic energy of materials with misfitting inclusions. *Acta metallurgica*, **21**,571-573, (1973)

[5] R. Hill. A self-consistent mechanics of composite materials, *J. Mech. Phys. Solids*. **13**, 213-222, (1965).

[6] Shao-Yun Fu, Bernd Lauke, Yiu-Wing Mai. *Science and engineering of short fibre reinforced polymer composite.* CRC Press, Boston New York, 2009.

[7] J.L. Thomason. The influence of fibre length and concentration on the properties of glass fibre reinforced polypropylene: Injection moulded long and short fibre PP, *Composites*, **A 33**,1641-1652, (2002).
[8] J.L. Thomason. The influence of fibre length and concentration on the properties of glass fibre reinforced polypropylene: 1. Tensile and flexural modulus, *Composites*, **A 27**, 477-484, (1996).