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Numerical investigation of thermal and thermo-mechanical effective properties for short fibre reinforced composite

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Abstract This study aims to investigate the thermal conductivity and the linear coefficient of thermal expansion for short fibre reinforced composites. The study combines numerical and statistical analyses in order to primarily examine the representative size and the effective properties of the volume element. Effects of various micromechanical parameters, such as fibre's aspect ratio and fibre's orientation, on the minimum representative size are discussed. The numerically acquired effective properties, obtained for the representative size, are presented and compared with analytical models.

Keywords RVE · homogenisation · stochastic parameters · short fibre reinforced composites

1 Introduction

Increasing number of processing cycles in polypropylene, injection moulded or extruded can cause a severe degradation of the molecular weight of the polymer [1]. As a consequence, properties such as Youngs modulus, strength and elongation at break, are highly affected by the recycling process: e.g. modulus of elasticity increases as the number of processing operations increase for extruded polypropylene, while modulus decreases as the number of processing operations increase for injection moulded samples. It is thus, characterisation of short fibre reinforced composite has attracted a lot of interest recently. Various approaches have been reported regarding numerical ([2,3,4,5,6,7]), experimental ([8]) and analytical characterisation of SFRC. Building upon our earlier study the analyses of micro-mechanical parameters of SFRCs [9], [10] this study continues exploring the topic in order to widen it to the thermal and thermo-mechanical classes of problems. This paper aims at characterising and, perhaps, generalising and extending the existing knowledge of the thermal and thermo-mechanical properties of a SFRC through a combined numerical and statistical approach. A general methodology is presented in the paper, with emphasis being put on materials microstructural geometrical properties such as fibres aspect ratios and fibres orientations and their influence on the effective proprieties of a composite material.

2 Methodology

This section presents the methodology used to define the effective thermal and thermo-mechanical properties of a composite material. A generic description of this methodology is based on the concept of a Representative Volume Element [11]. RVE is widely used in numerical mechanics: various multi-scale methodologies often use this concept, condition to the separation of scales principle being fulfilled. Further links of an RVE to a length-scale parameter of a material can be found in [12] in the framework of gradient elasticity [13] and gradient

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viscoelasticity [14]. RVE concept not only can be used in man-made composite material, natural material, e.g. bones are often described using this concept (see, among others [15, 16, 17, 18]).

Main steps of the methodology adopted here, to define an RVE are outlined below for readers benefit:

1. identify a starting size of a unit cell and for this size create a micro-structure with specific geometrical characteristics (e.g. in this paper fibre orientation and aspect ratio are of interest);
2. in this unit cell solve particular boundary-value problem;
3. define homogenised solution for the analysed unit cell;
4. perform a statistical analysis to recover *effective* properties, (e.g. using the chi-square goodness of fit statistical test);
5. following the results of the statistical analysis in the previous step, make a decision whether the unit cell size under investigation is representative, alternatively increase the unit cell size and start again.

The whole process is repeated for all possible combinations of different micro-mechanical geometrical parameters: three aspect ratios and three cases of fibres orientation are analysed. In the following subsections the aforementioned steps will be analysed in more details.

2.1 Step 1: Creation of the microstructure

In order to create a reliable numerical representation of SFRC micro-structure, two conditions should be satisfied: (i) The packing problem should be solved, and (ii) periodicity of the material should be enforced.

Packing problem is a class of optimisation problems in mathematics that attempts to pack objects together in a (volume) container by satisfying various constrains. The difficulty of solving the packing problem in SFRCs arises due to the influence of fibre orientation (FO) and fibre aspect ratio (AR) (see Figures 1a, 1b and [9] for the details). The geometric periodicity [19] implies that each inclusion within the boundaries of the unit cell *reappears* on the opposite side of the square unit, thus ensuring the geometric continuity of a material.

Taking into consideration conditions of packing and periodicity, the material's microstructural geometry has been created with MatLab software and introduced to Abaqus 6.10-2 commercial FE package through Python scripting. Fibres have been modelled as elliptical shapes partitioned from a continuous matrix with different mechanical and thermal properties. The interphase between matrix and fibres was assumed perfect. Two dimensional triangular elements (Abaqus: $DC2D3$ and $CPE3T$) have been used for the thermal conductivity and coefficient of thermal expansion correspondingly.

2.2 Step 2: Boundary value problem

In order to study the effective thermal conductivity of the composite microstructure, a temperature difference was applied on the opposing sides of the unit cell, with the remaining sides subjected to adiabatic boundary conditions. A constant temperature (T_{Low} and T_{High}) was applied on the left (L), right (R), top (T) and bottom (B) edges of the unit cell. Equations (1a) to (1d) indicate the applied boundary conditions for calculating thermal conductivity. In order to calculate the coefficient of thermal expansion, the kinematic degrees of freedom were restricted on the perimeter of the square, while a temperature difference was applied between the opposite edges.

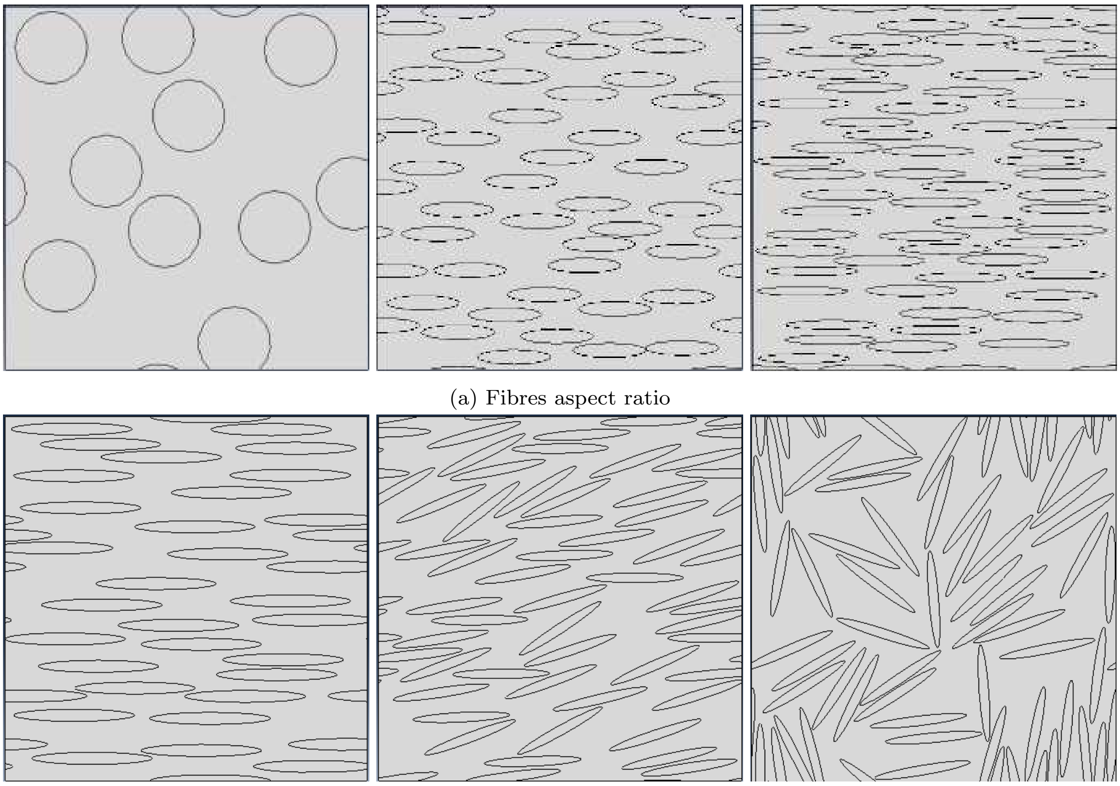
$$\boldsymbol{T}^{(L)} = \boldsymbol{T}_{Low},\ \boldsymbol{T}^{(R)} = \boldsymbol{T}_{High} \tag{1a}$$

$$\boldsymbol{T}^{(B)} = 0,\ \boldsymbol{T}^{(T)} = 0 \tag{1b}$$

$$\boldsymbol{u}^{(L)} = \boldsymbol{u}^{(R)} = 0 \tag{1c}$$

$$\boldsymbol{u}^{(T)} = \boldsymbol{u}^{(B)} = 0 \tag{1d}$$

As a consequence of the temperature difference a heat flux occurred from the high temperature bound towards the low temperature. Local heat flux was measured in every integration point of all finite elements. The developed stress field due to the thermal expansion of the composite material is measured from all the integration points of each element.



(a) Fibres aspect ratio

(b) Fibres orientations

Fig. 1: Geometrical characteristics

2.3 Step 3: Homogenised solution

The overall goal of micro-mechanical computations is to, eventually, produce more accurate and detailed response that is associated with the considered material sample. In other words the aim is to produce *effective* and microstructure driven (versus somewhat phenomenologically introduced) properties of the considered material. One of the approaches to determine these effective properties is through the process of homogenisation. As such, a volume average homogenisation approach was applied on the data obtained in the previous step (Section 2.2) in each considered unit cell, such that the total averaged heat flux $\bar{q}$, associated with the current unit cell of volume $\boldsymbol{V}$, is now defined through

$$\bar{\boldsymbol{q}} = \frac{1}{\boldsymbol{V}} \int_{\Omega} \boldsymbol{q} d\boldsymbol{V} \tag{2}$$

In order to calculate the effective thermal conductivity, Fouriers law for thermal conductivity is used. The time dependent function of Fouriers law is shown in Equation (3).

$$\nabla(\boldsymbol{K}\nabla\boldsymbol{T}) = \rho C_p \frac{\partial \boldsymbol{T}}{\partial t} \tag{3}$$

here ρ and C_P represent density of the material and specific heat correspondingly. For the purpose of this research, thermal conductivity has been investigated for the steady – state condition. The steady – state condition describes the response of the material in terms of thermal conductivity, once dynamic phenomena that occur through the heat transfer process are constant. The steady – state version of Fouriers thermal conductivity law are shown in Equation (4).

$$\boldsymbol{q} = \boldsymbol{K} \frac{\partial \boldsymbol{T}}{\partial \boldsymbol{x}} \tag{4}$$

With known temperature difference and the length of the unit cell, the thermal conductivity for the longitudinal and transverse directions can be defined as:

$$\begin{Bmatrix} q_x \\ q_y \\ q_z \end{Bmatrix} = \begin{bmatrix} K_{xx} & K_{xy} & K_{xz} \\ K_{yx} & K_{yy} & K_{yz} \\ K_{zx} & K_{zy} & K_{zz} \end{bmatrix} \begin{Bmatrix} \partial T/\partial x \\ \partial T/\partial y \\ \partial T/\partial z \end{Bmatrix} \tag{5}$$

The average stress was obtained using Equation (6)

$$\bar{\boldsymbol{\sigma}} = \frac{1}{\boldsymbol{V}} \int_{\Omega} \boldsymbol{\sigma} d\boldsymbol{V} \tag{6}$$

and the calculated values for the stiffness were used in order to define longitudinal and transverse coefficient of thermal expansion:

$$\bar{\boldsymbol{\sigma}} = \boldsymbol{C}(\boldsymbol{\varepsilon} + \boldsymbol{\alpha} \triangle \boldsymbol{T}) \tag{7}$$

here $\bar{\boldsymbol{\sigma}}$ represents the average stress while $\boldsymbol{\sigma}$ refers to the local stress in each integration point.

During the calculation of the effective coefficient of thermal expansion, the macro–strain values $\boldsymbol{\varepsilon}$ are equal to zero due to the restriction in kinematic boundary conditions. Effective stiffness tensor has been evaluated from the pure mechanical homogenisation process, and the same values were used for solving the thermo–mechanical problem.

2.4 Steps 4 and 5: Statistical analysis and effective properties

In this step, numerical tests for all the possible combinations of considered aspect ratios and fibre orientations were performed[1]. A brief explanation on the statistical test will follow. For further details please see earlier literature [19], [9] about the statistical analysis used in this work. A hypothesis that a representative unit cell size is not sensitive to any spacial position or orientation of fibres in the micro-structure has been tested using a chi-square test. Tested samples, that passed the chi-square test, are considered to be representative (size is big enough) and thus suitable for obtaining homogenised solution (see Section 2.3) and are defined as *effective*. For each case of aspect ratio and fibre orientation, combinations of five different realisations were developed (see Figure 2). A hypothesis that the average calculated stiffness of five different realisations is not sensitive to any changes regarding the spacial position or the orientation of fibres has been tested using a chi-square test. Chi square test was used as expressed through equation (8). Note that for the current study the critical value of the chi-square test was calculated based on the accuracy of 97.5 in combination with 3 degrees of freedom. Also it must be noted that all the values entering the test have been normilised in respect with the higher value and lay between the open interval of $1 - 10$. This allow a direct comparison between the chi-square results of every tested combination of aspect ratio, fibre orientation and size.

$$\chi^2 = \sum_{j=1}^{NoE} \frac{(O_j - E_j)^2}{E_j} \tag{8}$$

Where $\O_j$ and E_j represents the observed and expected value, NoE represents the Number of Elements

3 Results and discussion

Following the procedure, introduced in Section 2, microstructural samples-realisations have been constructed. Mechanical, thermal and thermo-mechanical properties of composite material's component have been kept same in all tests. Table 1 presents these properties:

[1] In this paper the volume fraction of fibres 30% is assumed

Fig. 2: Geometrical realisations of the microstructure

Table 1: Mechanical properties used for the constituent materials in this study

Property	Glass fibres	Polypropylene
Thermal Conductivity [W/mK]	0.05	0.15
Coefficient of Thermal Expansion [m/mK]	4.3×10^{-6}	86.4×10^{-6}
Young's modulus [GPa]	$72\ GPa$	$1.2\ GPa$
Poisson ratio	0.21	0.335

3.1 Numerical results

The statistical results including chi-square values are presented in Table 2. Thermal conductivity and coefficient of thermal expansion values are used separately in further analysis.

Table 2: Statistical data for analysed properties

Property	Orientation	Unit cell size	Aspect Ratio 1	Aspect Ratio 5	Aspect Ratio 10
Thermal Conductivity	Aligned	2.5	0.02	0.013	0.015
		3.75	0.003	0.001	0.005
		5.0	0.0003	0.003	0.0041
	Misaligned	2.5		0.092	0.0007
		3.75		0.0019	0.00031
		5.0		0.0004	0.00035
	Random	2.5		0.041	0.053
		3.75		0.026	0.012
		5.0		0.0047	0.003
Coefficient of Thermal Expansion	Aligned	2.5	2.31	0.53	0.521
		3.75	0.75	0.29	0.297
		5.0	0.34	0.04	0.078
	Misaligned	2.5		0.355	1.01
		3.75		0.1675	0.335
		5.0		0.1192	0.273
	Random	2.5		0.6681	1.09
		3.75		0.5356	0.6835
		5.0		0.131	0.117

Chi-square test is a hypothesis test used to verify that the conclusion in the effective properties is up to a percentage accurate for the effective properties under study. The critical value for passing or not the test was obtained from the chi-square table by considering 3 degrees of freedom and 97.5 accuracy. Degrees of freedom where calculated based on equation (9). Considering the aforementioned tests with obtained chi-square values (see Table 2) smaller than the table value of 0.025, can be considered as successful unit cell sizes able to represent the homogenised structure. The stiffness tensor can be regarded as effective stiffness.

$$DoF = NoR - EP - 1 \tag{9}$$

Where: DoF are the degrees of freedom NoR are the number of realisations and PE are the estimated parameters

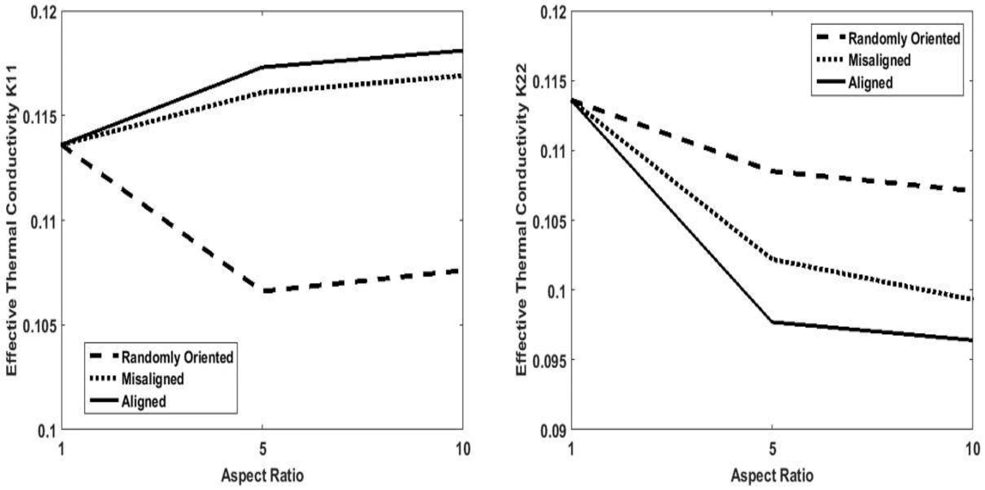
Results presented in Table (2) show that for higher aspect ratio, chi-square value has the tendency to decrease. More clear behaviour of the chi-square results, was observed in respect with the size. As long as the size increase the chi-square value decreases, which means that the observed results are closer to the expected values. Regarding the increases of the geometric randomness in orientation, seems that increase of the level of randomness increases the value of chi-square. The above characteristics were observed for both properties, thermal conductivity and coefficient of thermal expansion. Comparing results with respect to the effective property under investigation, it is clear that chi-square values for thermal conductivity are closer to each other for all parameters (aspect ratio, size, orientation). Last but not least it must be underlined that for the coefficient of thermal expansion the test indicate that higher sizes need to be considered. Sizes higher than five times the inclusion length are needed in order to get representative results for a composite with such a degree of inhomogeneity and such a geometry of the microstructure. On the other hand for the coefficient of thermal expansion even the smallest considered size is big enough to provide representative results.

Figure 3a shows numerical results for the effective thermal conductivity. Results are presented for size equal to 3.75 times inclusion's length. Effective properties were plotted in respect with the aspect ratio for different orientation. As it can be noted from Figure 3a longitudinal and transverse conductivity follow the opposite trend in respect to orientation. Aligned fibres exhibit the highest thermal conductivity followed by the misaligned fibres and the less conductive randomly oriented fibres. Regarding the thermal conductivity on the transverse direction, randomly oriented fibres are the most conductive followed by misaligned fibres and aligned fibres. Regarding the longitudinal thermal conductivity, while aspect ratio increases thermal conductivity in longitudinal direction increases as well with the exception of randomly oriented fibres. This may be due to the fact that randomly oriented fibres act as a barrier on the head flow as fibre's material is less conductive than the matrix . This can be enhased by noticing the distribution of thermal conductivity on the transverse direction with respect to fibre's orientation. The case of aligned fibres (which geometrically lies perpendicular to the heat flow) shows the smallest thermal conductivity with misaligned and randomly oriented fibres to follow. It is becoming clear that once the fibres are oriented perpendicular to the direction of heat flow, (for example: transverse conductivity on aligned fibres) the material is becoming less conductive as fibre's material is less conductive and act as a barrier on the heat flow. This can be concluded for the contribution of both parameters (aspect ratio and orientation)

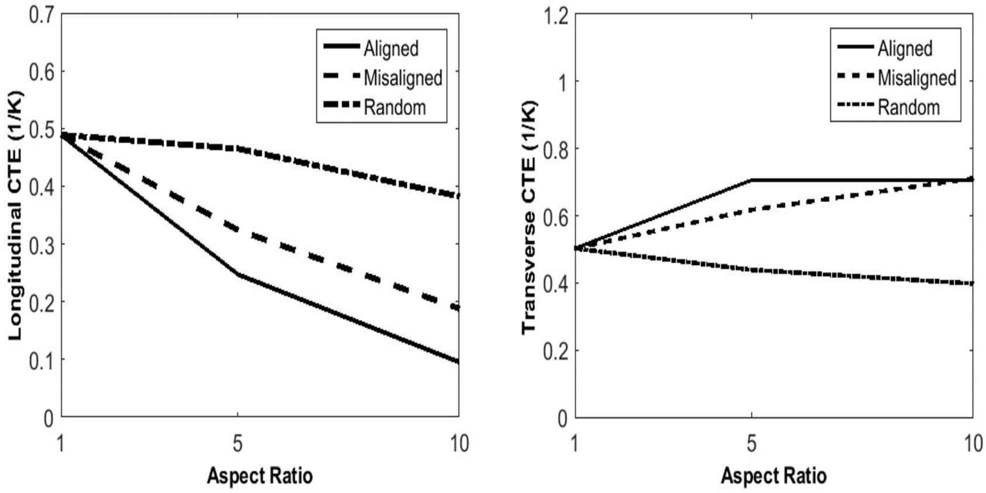
Figure 3b shows the effective longitudinal and transverse coefficients of thermal expansion For the longitudinal CTE randomly oriented fibres show the higher coefficient followed by the misaligned fibres and the randomly oriented fibres. The coefficient of thermal expansion decrease with respect to the increase in aspect ratio. Circular inclusions and randomly oriented fibres produce higher CTE. The opposite trend was observed for the transverse coefficient: for the transverse direction aligned fibres have the higher CTE followed by misaligned and randomly oriented fibres. Regarding the contribution of aspect ratio, CTE increases with respect to the increase of aspect ratio with an exception of randomly oriented fibres. It must be underlined that according to the statistical analysis and the chi-square results, transverse CTE for misaligned fibres is not considered as representative and any conclusions about the results are meaningless.

3.2 Comparison of the results with analytical models

Developed models for calculating thermal conductivity and coefficients of thermal expansion have been compared with predictions of Nielsen's model in the case of thermal conductivity and Schapery's model in the case of coefficient of thermal expansion. For the reader's benefit short introductions into Nielsen and Schapery's models are listed below.



(a) Effective thermal conductivity



(b) Effective coefficient of thermal expansion

Fig. 3: Left: Effective Thermal Conductivity, Right: Effective Coefficient of Thermal Expansion

Nielsen model Nielsens model [20] is a similar approach to Halpin's methodology [21], however Nielsens model includes a parameter which accounts for the packing arrangement through the maximum achievable volume fraction. Longitudinal and transverse thermal conductivity of aligned composite can be predicted through Equation (10) and Equation (11) respectively:

$$K_1 = \frac{1 + 2(L/d)\xi_1 V_f}{1 - \xi_1 \psi V_f} K_m \tag{10}$$

$$K_2 = \frac{1 + 0.5\xi_2 V_f}{1 - \xi_2 \psi V_f} K_m \tag{11}$$

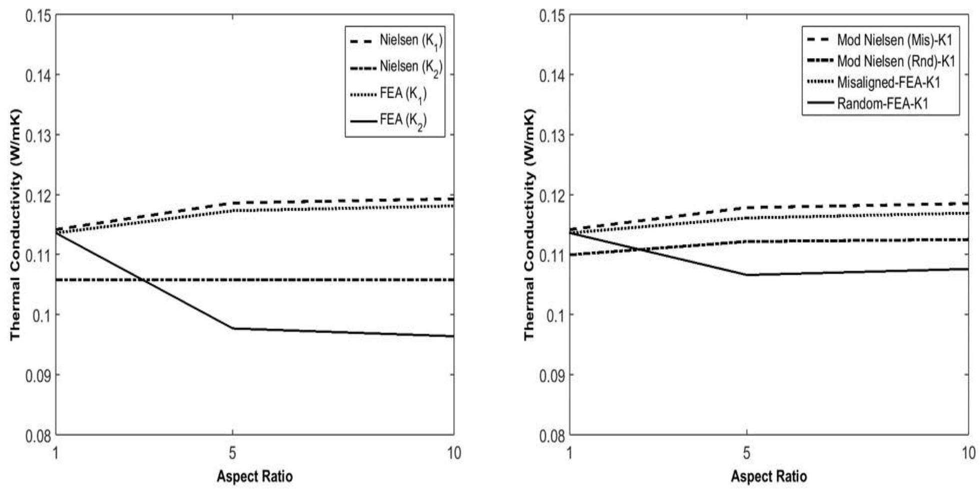
For the above equations parameters ξ_1, ξ_2 and ψ take values resulting from

$$\xi_1 = \frac{K_{f1}/K_m - 1}{K_{f1}/K_m + 2L/d} \tag{12}$$

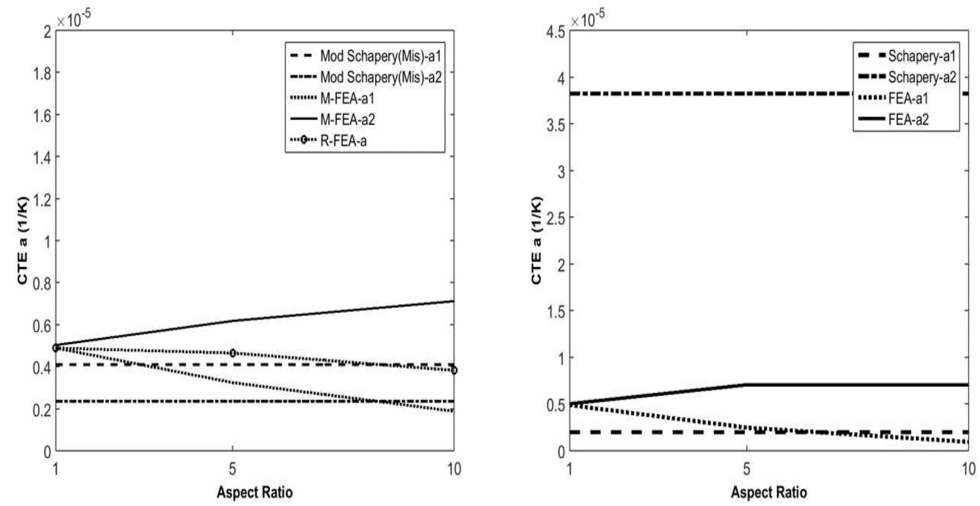
$$\xi_2 = \frac{K_{f1}/K_m - 1}{K_{f1}/K_m + 0.5} \tag{13}$$

$$\psi = 1 + \frac{1 - V_{f(\max)}}{V_{f(\max)}^2} V_f \tag{14}$$

The value of the parameter ψ is strongly dependant on the maximum achievable volume fraction which is strongly affected by the dispersion state and the shape of the fillers. Parameters ξ_1 and ξ_2 are the parameters of the model which reflect information of the geometry of the reinforcement and the degree of inhomogeneity in the composite material.



(a) Thermal conductivity



(b) Coefficient of thermal expansion

Fig. 4: Comparison between numerical and analytical predictions. Left - aligned fibres and right - misaligned and random fibres

Schaperys model An analytical model to calculate longitudinal and transverse coefficients of thermal expansion is Schaperys model [22]. Schapery's based his approach on an iso-strain behaviour of fibres and matrix. Equation (15) and Equation (16) show the calculation of longitudinal and transverse coefficients of thermal expansion in Schaperys model:

$$\alpha_l = \frac{E_f \alpha_f V_f + E_m \alpha_m V_m}{E_f V_f + E_m V_m} \tag{15}$$

$$\alpha_t = (1 + \nu_f)\alpha_f V_f + (1 + \nu_m)\alpha_m V_m - \alpha_l(\nu_f V_f + \nu_m V_m) \tag{16}$$

where in the above equation ν_f and ν_m represent Poisson's ratios for the fibres and matrix respectively, while α_l and α_t stand for the longitudinal and transversal CTE of the composite.

Nielsen and Schapery's models were used for aligned fibres. For the case of misaligned and random fibre orientations response were compared with the modified models of Nielsen and Schapery. The modified Nielsen's and Schapery's models, were properly modified in order to consider any degradation of the elastic properties due to the fibre's orientation. The degradation due to randomness on fibres orientation is applied as factors-multipliers on the calculated longitudinal and transverse elastic stiffness.

Figure 4 shows the comparison between analytical models prediction and results from the numerical models. As it can be seen numerical predictions are close to the analytical results. The comparison seems to experience the major deviation regarding the CTE and thermal conductivity for aligned fibres. The influence of random or misaligned orientation was captured evenly in both models. Both analytical and numerical results indicate that the influence of aspect ratio (up to aspect ratio=10) is small, especially with regard to thermal conductivity. Analytical and numerical predictions for CTE show more compliance behaviour regarding changes in aspect ratio and orientation.

4 Conclusions

In this paper an analysis of thermal and thermo-mechanical characteristics in thermoplastic short fibre composite has been performed. A methodology to create and numerically test heterogeneous microstructure has been presented together with illustrative examples in order to demonstrate the technique to calculate the effective properties of the composite. Influences of geometrical characteristics, such as aspect ratio and orientation of fibres in short fibre composite material, on the overall effective properties have been studied. Interestingly, a very low influence of aspect ratio on the effective properties was observed.

Additionally, opposite trends were observed for the longitudinal and transverse thermal conductivity values, and the orientation of the fibres: in general, the longitudinal thermal conductivity in the aligned fibres showed more conductive behaviour, while for the transverse effective thermal conductivity, the randomly oriented fibres showed a more conductive response. The results for the misaligned oriented fibres lay somewhat in between the aligned and randomly oriented fibres.

Analysing the effective coefficient of thermal expansion, a strong influences from both aspect ratio and fibre orientation were observed. More specifically, the transverse effective coefficient of thermal expansion increased by increasing the aspect ratio, where the opposite trend was observed for the effective longitudinal coefficient of thermal expansion. As it was mentioned above, the effective thermal conductivity also showed a strong dependency on the fibre orientation. For the effective transverse coefficient of thermal expansion, the aligned fibres produced higher effective values, while the misaligned and randomly oriented fibres exhibited lower coefficient of thermal expansion respectively.

In the longitudinal effective coefficient of thermal expansion once again the opposite trend was noted: randomly oriented and misaligned fibres exhibited the higher coefficient of thermal expansion while aligned fibres exhibited much lower CTE.

Finally numerical tests have been compared with the available analytical models. The results show that numerical results are in between the generic bounds of Voigt and Reuss predictions and in most cases aligned with the analytical models.

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