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A regression-based model for the transverse coefficient of thermal expansion of composites

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Abstract: It is important to correctly predict the coefficient of thermal expansion (CTE) in the design and analysis of fiber reinforced composite structures. Since the CTE for polymer resin materials is typically much higher than for fibers, and fibers often exhibit anisotropic thermal and mechanical properties, the stress induced in the composite due to temperature change is very complex. Both analytical and numerical methods have been developed to predict the transverse CTE of composites. It is seen that large discrepancies exist among different analytical models developed over the years. The accuracy of numerical methods such as finite element analysis has been proved in various studies. However, they are inconvenient for practical applications because of the complicated and time-consuming pre-processing, computation and post-processing processes. In this study, a transverse CTE model for composites was developed based on finite element analysis (FEA) and regression.

First, a three-dimensional steady state FEA model was developed to calculate the transverse CTE of composites. With the consideration of the Poisson effect of the resin, the micromechanical model was assumed to be $\alpha_{22} = \alpha_m(1+\nu_m) + \lfloor \alpha_{fT} - \alpha_m(1+\nu_m) \rfloor \beta$ (Dong 2008), where β is a function of V_f to be determined. In order to describe the behavior of the transverse CTE vs. the fiber volume fraction, an equation consisting of location parameter a_0, shape parameter a_1 and longitudinal constraint parameter a_2 was introduced as $\beta = a_0 V_f^{a_1} + \dfrac{a_2}{V_f}$.

Second, a factorial design was employed to study the influences of the constituent properties on the transverse CTE. The results show that the significant factors for both a_0 and a_1 are E_{fT}/E_m, ν_m and ν_{fTT}, and those for a_2 are E_{fT}/E_m, α_{fT}/α_m and ν_m. a_0 increases with E_{fT}/E_m and ν_{fTT} and decreases with ν_m; on the contrary, a_1 increases with ν_m and decreases with E_{fT}/E_m and ν_{fTT}. a_2 decreases with E_{fT}/E_m and increases with α_{fT} and ν_m. The results also show that E_{fL}/E_{fL}^0 is significant and a_2 decreases with E_{fL}/E_{fL}^0. The Analysis of Variance (ANOVA) also indicates that since significant curvature exists, a linear model is not sufficient.

Finally, a regression model was developed. Since it was found that a linear model was not sufficient, additional data points were collected by the central composite design (CCD) (Montgomery 2000). In addition, the data of glass/epoxy composites was included in the model development. The regression model was based on a combination of Michaelis-Menten and linear models. By using Least Squares Estimation (LSE), the coefficients were fitted as:

$$a_0 = \left(1.08 + \frac{0.15}{12.02 - E_{fT}/E_m}\right)\left(0.97 - 0.15\nu_m + 0.015\nu_{fTT}\right)$$

$$a_1 = \left(0.19 + \frac{3.23}{29.79 + E_{fT}/E_m}\right)\left(2.67 + 2.01\nu_m - 0.23\nu_{fTT}\right)$$

$$a_2 = 0.001\left(0.44 + \frac{28.96}{60.11 + E_{fT}/E_m}\right)\left(-0.22 + 0.94\,\alpha_{fT}/\alpha_m + 3.33\nu_m\right)\left(E_{fL}/E_{fL}^0\right)^{-0.69}$$

The model was validated against the FEA and experimental data. It shows that the model presented in this paper offers excellent accuracy without complicated numerical modeling process.

Keywords: *composite, coefficient of thermal expansion, transverse, regression*

1. INTRODUCTION

Fiber reinforced composite materials have been widely used due to their advantages over traditional materials including high stiffness to weight ratio, excellent durability and design flexibility. Thermal expansion is an important aspect in the design and analysis of composite structures since composites are usually processed at an elevated temperature and residual stresses are induced due to the temperature. Thus, the coefficients of thermal expansion (CTE) of composites need to be correctly predicted.

Since the CTE for polymer resin is typically much higher than for fibers, and fibers often exhibit anisotropic thermal and mechanical properties, the stress induced in the composite due to temperature change is very complex. A number of analytical models have been developed for the CTE of unidirectional composites (Chamberlain 1968; Schapery 1968; Hashin 1979; Chamis 1984; Bowles and Tompkins 1989; Sideridis 1994; Stellbrink 1996), based on simple rule of mixtures to thermoelastic energy principles. However, large discrepancies exist among different models for the transverse CTE. These analytical models were compared with the experimental measurements and FEA by Bowles and Tompkins (Bowles and Tompkins 1989). The results show that FEA is accurate in calculating the effective CTE of composites. Other studies (Islam et al. 2001; Karadeniz and Kumlutas 2007) have also shown similar results.

In this study, the transverse CTE of composites were calculated by FEA using a representative unit cell. The significant factors affecting the transverse CTE were identified by Design of Experiments (DOE) (Montgomery 2000). A regression-based model for predicting the transverse CTE of composites was developed and validated against the FEA and experimental data.

The advantage of the model presented in this paper is that no complicated numerical modeling process is needed. Thus, this model is potentially useful for the design of composite components and assemblies by correctly predicting of the residual stresses or thermal stresses, since these stresses are directly dependent on the CTE. The potential applications of this model include design optimization, failure prediction, etc.

2. FINITE ELEMENT ANALYSIS

It is seen from the literature that FEA has been proved to offer better accuracy than analytical models. Thus, in this study, an FEA model using a representative unit cell was first developed to calculate the CTE of composites. The finite element formulation assumes that a condition of generalized plane strain exists in the unidirectional composites.

For convenience, the fibers were assumed to be in hexagonal arrays, since the fiber packing had little effect on the CTE (Dong 2008). A representative unit cell is as shown in **Figure 1**. Three dimensional steady state analyses were employed to calculate the effective CTE. The commercial FEA package MSC.Marc Mentat (MSC Software Corporation, Santa Ana, CA) was employed in this study. By applying symmetric boundary conditions, only one quarter of the unit cell was modeled in FEA. After meshing, the mechanical and thermal properties for both the fibers and the resin were input. The boundary conditions used in FEA were as follows: along the planes *x*, *y*, and *z* = 0, the model was restricted to move in the *x*, *y*, and *z* directions, respectively. Along the opposite planes, the nodes were constrained so that they had the same normal displacement. This was achieved by defining links in MSC.Marc Mentat. The model underwent a unit temperature drop. The CTE in the *x*, *y*, and *z* directions were obtained respectively. The grid convergence was tested to ensure sufficient accuracy. As an example, the transverse CTE of AS4 graphite/epoxy composites were calculated by FEA. For comparison, it was also calculated by Schapery and Chamis models, which are two commonly used analytical models. V_f was varied from 1% to the maximum (90.69%). The results are as shown in **Figure 2**. It is shown that Schapery model overestimates the transverse CTE, and the relative difference from FEA can be as high as 10%, while Chamis model significantly underestimates the transverse CTE, and the relative difference can be as high as 30%. Thus, these analytical models are inaccurate in predicting the transverse CTE of composites.

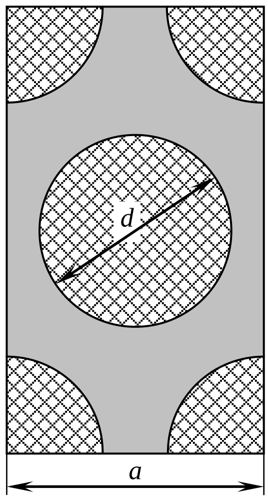

Figure 1. Construction of a representative unit cell

Figure 2 also shows that the transverse CTE decreases with the fiber volume fraction except at lower fiber volume fractions. The maximum of the transverse CTE occurs at approximately V_f = 5%. This is due to the strong longitudinal constraint exerted by the fibers. Because the longitudinal CTE of fibers is much lower, the resin is squeezed out in the transverse direction. Thus, at lower fiber volume fractions, the transverse CTE is higher than the CTE of pure resin.

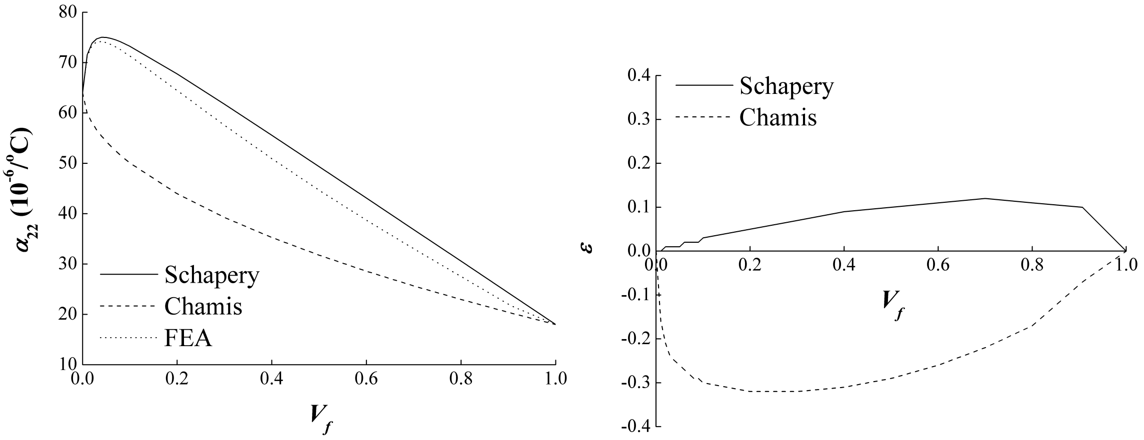

Figure 2. Left: transverse CTE of AS4 graphite/epoxy composites calculated by FEA and analytical models; right: relative errors of analytical models

In this study, with the consideration of Poisson effect of the resin, the micromechanical model was assumed to be in the form as follows (Dong 2008):

$$\alpha_{22} = \alpha_m(1+\nu_m) + \lfloor \alpha_{fT} - \alpha_m(1+\nu_m) \rfloor \beta \tag{1}$$

where β is a function of V_f to be determined.

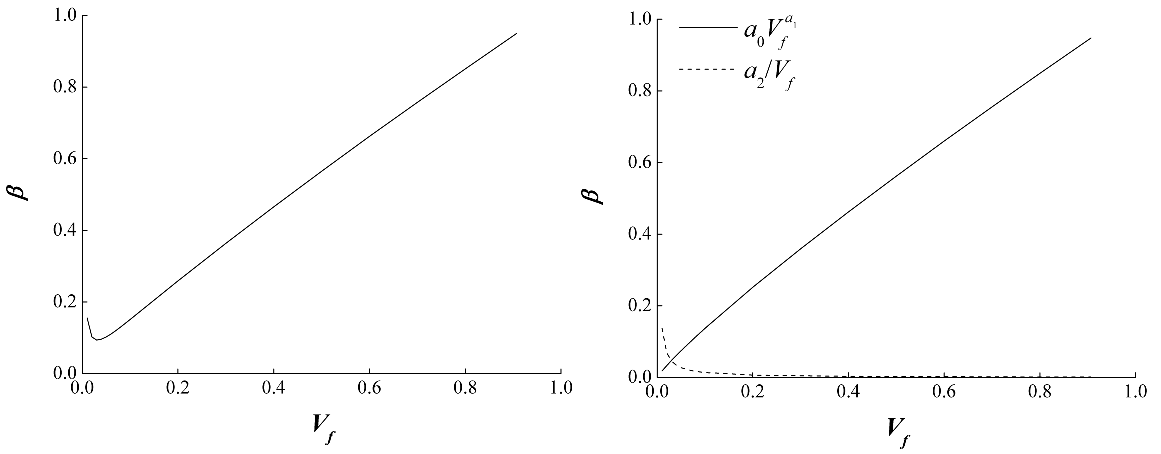

Figure 3. Left: β vs. V_f; right: decomposition of β–V_f curve

The transverse CTE calculated from FEA were converted into β. The range of β is 0 to 1. As shown in **Figure 3**, β can be represented by the combination of a power function and a reciprocal function of V_f, i.e.

$$\beta = a_0 V_f^{a_1} + \frac{a_2}{V_f} \tag{2}$$

where a_0 and a_1 are the location and shape parameters, respectively; and a_2 is called the longitudinal constraint parameter, which represents the strong longitudinal constraint effect exerted by the fibers at lower V_f.

3. MODEL DEVELOPMENT

3.1. Identification of significant factors

First, a factorial design was employed to study the influences of the constituent properties on the transverse CTE. Factorial designs are most efficient for experiments involving the study of the effects of two or more factors. In a factorial design, all possible combinations of the levels of the factors are investigated. Thus, it allows studying the effect of each factor on the response variable, as well as the effects of interactions between factors on the response variable (Montgomery 2000).

For the transverse CTE of composites, the responses were chosen to be a_0, a_1 and a_2, and the transverse factors E_{fT}, α_{fT}, ν_{fTT}, E_m, α_m and ν_m were initially considered. In order to reduce the number of factors, dimensionless variables E_{fT}/E_m, α_{fT}/α_m, ν_m and ν_{fTT} were derived, with E_m and α_m fixed at 2581 MPa and 6.4×10^{-5}/°C. The ranges of E_{fT} and α_{fT} were chosen so that most carbon fibers were included. Both ν_m and ν_{fTT} were varied between 0.2 and 0.4. The levels of chosen factors are as shown in Table **1**.

A full 2^4 factorial design with center point was employed. The data were analyzed using Design-Expert® software (Stat-Ease, Inc. Minneapolis, MN). The results show that the significant factors for both a_0 and a_1 are E_{fT}/E_m, ν_m and ν_{fTT}, and those for a_2 are E_{fT}/E_m, α_{fT}/α_m and ν_m. a_0 increases with E_{fT}/E_m and ν_{fTT} and decreases with ν_m; on the contrary, a_1 increases with ν_m and decreases with E_{fT}/E_m and ν_{fTT}. a_2 decreases with E_{fT}/E_m and increases with α_{fT} and ν_m. The Analysis of Variance (ANOVA) also indicates that since significant curvature exists, a linear model is not sufficient.

Because of the strong longitudinal constraint exerted by the fibers at low fiber volume fractions, a_2 is also dependent on the longitudinal properties of fibers. With the transverse properties fixed at the center point, the influence of E_{fL}/E_{fL}^0 and α_{fL}/α_m, was investigated by a 2^2 factorial design with center point as shown in Table **2**. The results show that E_{fL}/E_{fL}^0 is significant and a_2 decreases with E_{fL}/E_{fL}^0.

Table **1**. Levels of dimensionless transverse factors

	Low	High
E_{fT}/E_m	2.7121	7.7489
α_{fT}/α_m	0.0781	0.3125
ν_m	0.2	0.4
ν_{fTT}	0.2	0.4

Table **2**. Levels of dimensionless longitudinal factors

	Low	High
$E_{fL}/E_{fL}^{0\,*}$	0.4	1.6
α_{fL}/α_m	-23.44×10^{-3}	-1.56×10^{-3}

* E_{fL}^0 = 500 GPa is the reference longitudinal elastic modulus of fibers

3.2. Model development

The significant factors identified were chosen to develop a regression model. Since it is concluded that a linear model was not sufficient, more data points were collected by the central composite design (CCD) (Montgomery 2000). In addition, the data of glass/epoxy composites was included in the model development.

The regression model was based on a combination of Michaelis-Menten and linear models. The introduction of Michaelis-Menten model is to account for the non-linearity. Michaelis-Menten model (Briggs and Haldane 1925) is a mathematical equation expressing the hyperbolic relationship between the initial velocity, V_0, and the substrate concentration, $[S]$, in a number of enzyme-catalyzed reactions, which reads

$$V_0 = \frac{V_{\max}[S]}{K_m + [S]} \tag{3}$$

where $V_{\max}$ is the maximum velocity and K_m is the Michaelis constant.

The complete data are as shown in Table **3**. By using Least Squares Estimation (LSE), the coefficients were fitted as:

$$
\begin{aligned}
a_0 &= \left(1.08 + \frac{0.15}{12.02 - E_{fT}/E_m}\right)\left(0.97 - 0.15\nu_m + 0.015\nu_{fTT}\right) \\
a_1 &= \left(0.19 + \frac{3.23}{29.79 + E_{fT}/E_m}\right)\left(2.67 + 2.01\nu_m - 0.23\nu_{fTT}\right) \\
a_2 &= 0.001\left(0.44 + \frac{28.96}{60.11 + E_{fT}/E_m}\right)\left(-0.22 + 0.94\,\alpha_{fT}/\alpha_m + 3.33\nu_m\right)\left(E_{fL}/E_{fL}^0\right)^{-0.69}
\end{aligned}
\tag{4}
$$

After the constituent properties and fiber volume fraction of a composite are known, the transverse CTE can be calculated by Eqns. 1-2 and 4.

Table **3**. Complete data set for regression analysis

E_{fT}/E_m	α_{fT}/α_m	ν_m	ν_{fTT}	a_0	a_1	a_2
2.7121	0.0781	0.2	0.2	1.0256	0.8924	0.5171
7.7489	0.0781	0.2	0.2	1.0457	0.8444	0.4581
2.7121	0.3125	0.2	0.2	1.0252	0.8921	0.6818
7.7489	0.3125	0.2	0.2	1.0453	0.8442	0.6204
2.7121	0.0781	0.4	0.2	0.9943	1.0047	1.0609
7.7489	0.0781	0.4	0.2	1.0150	0.9569	1.0214
2.7121	0.3125	0.4	0.2	0.9940	1.0054	1.2865
7.7489	0.3125	0.4	0.2	1.0144	0.9574	1.2473
2.7121	0.0781	0.2	0.4	1.0304	0.8720	0.4898
7.7489	0.0781	0.2	0.4	1.0475	0.8369	0.4462
2.7121	0.3125	0.2	0.4	1.0300	0.8717	0.6542
7.7489	0.3125	0.2	0.4	1.0468	0.8361	0.6106
2.7121	0.0781	0.4	0.4	1.0003	0.9847	1.0440
7.7489	0.0781	0.4	0.4	1.0173	0.9499	1.0152
2.7121	0.3125	0.4	0.4	0.9998	0.9853	1.2692
7.7489	0.3125	0.4	0.4	1.0166	0.9496	1.2399
5.2305	0.1953	0.3	0.3	1.0278	0.9014	0.8523
7.7489	0.3125	0.3	0.4	1.0346	0.8880	0.9493
7.7489	0.0781	0.4	0.3	1.0161	0.9532	1.0174
5.2305	0.3125	0.2	0.2	1.0390	0.8558	0.6368
2.7121	0.1953	0.4	0.2	0.9941	1.0049	1.1613
2.7121	0.3125	0.4	0.3	0.9969	0.9952	1.2769
5.2305	0.0781	0.2	0.4	1.0419	0.8450	0.4557
7.7489	0.0781	0.3	0.2	1.0334	0.8955	0.7570
2.7121	0.1953	0.2	0.4	1.0302	0.8719	0.5632
56.1798	0.0781	0.27	0.20	1.0011	0.7282	0.5084

4. MODEL VALIDATION

For the purpose of validation, first, the transverse CTE of AS4 graphite/epoxy composites was calculated by the developed model and FEA, respectively. V_f was varied from 1% to 96%. The result is as shown in **Figure 4**. Second, the model was validated against the FEA and experimental data for T300 graphite/934 composites from reference (Bowles and Tompkins 1989). The result is as shown in **Figure 5**. It can be seen from both cases that the relative error is within 2%. Thus, the current method is in excellent agreement with FEA.

5. CONCLUSIONS

In this study, the transverse CTE of fiber reinforced composites was calculated by finite element analysis using a representative unit cell. In order to describe the behavior of the transverse CTE vs. the fiber volume fraction, an equation consisting of location, shape and longitudinal constraint parameters was introduced. The significant factors affecting these parameters were identified by Design of Experiments (DOE). A regression-based model for predicting the transverse CTE was fitted to the data from FEA. The model was validated against the FEA and experimental data. It shows that the model presented in this paper offers excellent accuracy. The advantage of the model presented in this paper is that no complicated numerical modeling process is needed. Thus, this model is potentially useful for the design of composite components and assemblies by correctly predicting of the residual stresses or thermal stresses, since these stresses are directly dependent on the CTE. The potential applications of this model include design optimization, failure prediction, etc.

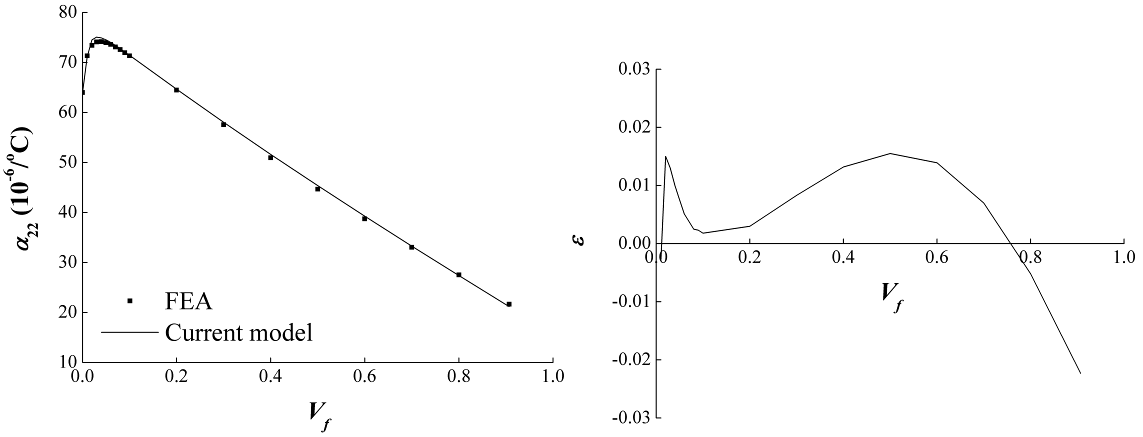

Figure 4. Left: transverse CTE of AS4 graphite/epoxy composites; right: relative error compared with FEA

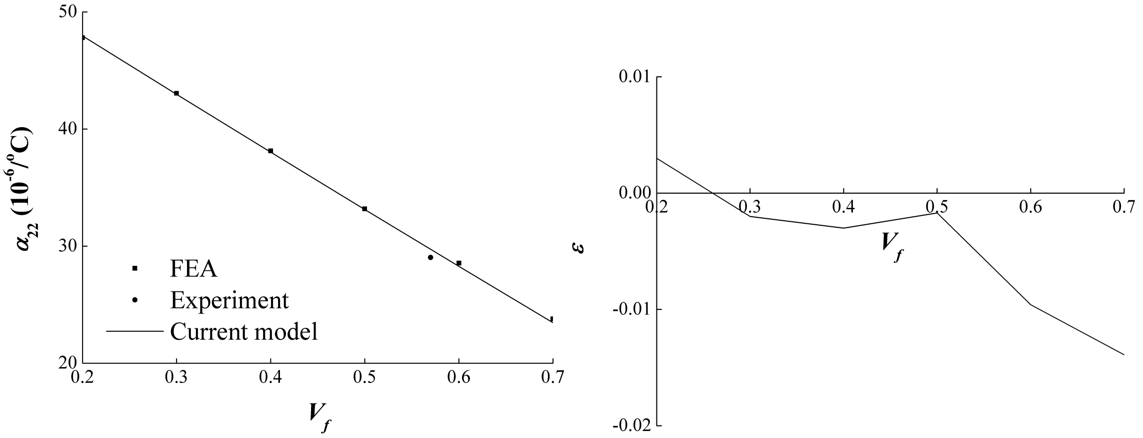

Figure 5. Left: transverse CTE of T300 graphite/epoxy composites; right: relative error of the current model compared with FEA

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Nomenclature

α_{11}	=	Longitudinal CTE of composite
α_{22}	=	Transverse CTE of composite
α_{fL}	=	Longitudinal CTE of fibers
α_{fT}	=	Transverse CTE of fibers
α_m	=	CTE of resin
E_{11}	=	Longitudinal modulus of composite
E_{22}	=	Transverse modulus of composite
E_{fL}	=	Longitudinal modulus of fibers
E_{fT}	=	Transverse modulus of fibers
E_m	=	Modulus of resin
G_f	=	Longitudinal-transverse shear modulus of fibers
G_{fTT}	=	Transverse-transverse shear modulus of fibers
G_m	=	Shear modulus of resin
ν_{12}	=	Longitudinal-transverse Poisson’s ratio of composite
ν_f	=	Longitudinal-transverse Poisson’s ratio of fibers
ν_{fTT}	=	Transverse-transverse Poisson’s ratio of fibers
ν_m	=	Poisson ratio of resin
V_f	=	Fiber volume fraction