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Modeling of residual stress appearance in the process of on-line consolidation of thermoplastic composites

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Abstract. On-line consolidation process is a promising non-autoclave technique to design large size parts in aeronautical industry. Residual stress growth during the process is locking significantly the process validation. Residual stress development results mainly first from the thermomechanical properties differences of the composite constituents and secondly from high thermal gradients occurring within the composite during the process. In this paper, we present a multi-scale modeling based on the Constrained Natural Element Method which takes into account material properties evolution during the process.

Keywords: numerical simulation, welding, composite, semicrystalline polymers, heat transfer, FEM, NEM, Karhunen-Loeve method, multi-scale calculation, homogenization.

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INTRODUCTION

Manufacturing of thermoplastic composites by on-line consolidation process is still not certificated in aeronautical industry. In this non-autoclave technique, the composite is manufactured progressively by fusion bonding a new prepreg layer to the previous one heating the interface and applying pressure [1]. In standard working conditions, parts realized with this type of process are subject to important residual stresses. The lack of knowledge on their origin and build up is locking significantly the validation of this promising process. The aim of this study is to develop a modeling procedure allowing predicting appearance of residual stresses within the composite during the on-line consolidation process. A schematic diagram of the on-line consolidation process and a modeling domain diagram representative of the phenomena occurring during the on-line consolidation process are displayed on Fig. 1.

FIGURE 1. Schematic diagram of the on-line consolidation process and a modeling domain diagram representative of the phenomena occurring during the process.

Residual stress development within the composite results mainly from two factors : first, the differences of the thermomechanical properties of the composite constituents, and secondly, the high thermal gradients occurring within the material. The evolution of material thermomechanical properties which occurs on microscopic scale must thus be taken into account in the modeling. A multi-scale modeling is therefore necessary.

In order to reduce time calculation and memory use, we must then define an equivalent homogeneous material for each microscopic cell.

NUMERICAL METHOD AND GOVERNING EQUATIONS

Crystallization and melting phenomena occurring in the composite during process due to welding fields cause important evolution of the material properties. These evolutions must be taken into account in the calculation, by using a multi-scale modeling.

We realize the multi-scale calculation as follow : microscopic and macroscopic computations are conducted in 2D dimension and by considering the material as thermoelastic. Macroscopic description is achieved by using polygonal finite element method [2]. Microscopic description is realized by employing constrained natural element method [3]. This method dismisses difficulties related to mesh by completing the whole estimation by means of nodal data.

Time scheme computations are performed using finished differences method with three time steps of the second order [4]. This method allows avoiding using too small time steps for the non-linear calculations.

Let us suppose that we have to describe microscopic and macroscopic state of the composite in the time interval $\{t_0, t_f\}$. We realize a partition of the time interval $\{t_0, t_f\}$ in m time intervals by means of a time step Δt_{Macro} :

$$t = t_0 + m \cdot \Delta t \quad . \quad (1)$$

We realize macroscopic calculation in each macroscopic time interval $\{t_0, t_0 + k \Delta t_{Macro}\}$ $k \in \{1, \dots, m\}$. For each macroscopic calculation we realize a set of p microscopic calculations in a temporal partition of p time steps Δt_{micro} . The principle of the temporal partition of the microscopic scale is given on Fig. 2.

FIGURE 2. Temporal partition of microscopic scale

Karhunen-Loeve method (or proper orthogonal decomposition) [5] is applied after each set of p microscopic calculations to reduce the number of equations. Then we resolve transfer scale tensors $[A(\underline{x}, \underline{X})]$ and $[B(\underline{x}, \underline{X})]$ linking respectively the microscopic representative volume element variables $\{\epsilon(\underline{x})\}$ and $\{\nabla T_{micro}(\underline{x})\}$, to the macroscopic variables $\{\epsilon(\underline{X})\}$ and $\{\nabla T_{Macro}(\underline{X})\}$. The application of the usual homogenization method [6] to the microscopic displacements and the thermal fields allows homogenizing mechanical and thermal properties of the material (Eq. 2) :

constitutive tensor $[C^{Hom}]$, thermal conductivity tensor $[k^{Hom}]$, thermal expansion tensor $\{\alpha^{Hom}\}$.

$$\left\{ \begin{array}{l} \{\epsilon(\underline{x})\} = [A(\underline{x}, \underline{X})] : \{\epsilon(\underline{X})\} \\ \{\nabla T_{micro}(\underline{x})\} = [B(\underline{x}, \underline{X})] : \{\nabla T_{Macro}(\underline{X})\} \end{array} \right\} \Rightarrow \left\{ \begin{array}{l} [C^{Hom}(\underline{X})] = \int_{\Omega_{micro}} [A(\underline{x}, \underline{X})] : [C_{micro}(\underline{x})] d\Omega \\ [k^{Hom}(\underline{X})] = \int_{\Omega_{micro}} [B(\underline{x}, \underline{X})] : [k_{mi}(\underline{x})] d\Omega \end{array} \right. \quad (2)$$

A schematic diagram of the multi-scale calculation algorithm is given on Fig. 3.

FIGURE 3. Schematic diagram of the multi-scale calculation algorithm.

Homogenized properties are then used in the macroscopic scale at next time increment. Thus we obtain microscopic and macroscopic descriptions of the composite during the whole process. Stress field can then be calculated everywhere in the composite by the equations :

$$\left\{ \begin{array}{l} \{\sigma(\underline{X})\} = [C^{Hom}(\underline{X})] : (\{\epsilon(\underline{X})\} - \{\epsilon^{th}(\underline{X})\}) \\ \{\epsilon^{th}(\underline{X})\} = \{\alpha^{th}(\underline{X})\} (T_{Macro}(\underline{X}) - T_{ref}) \end{array} \right. \quad (3)$$

Residual stress field within the composite can then be evaluated.

FIRST RESULTS

Using the above-described numerical method to simulate elementary tests, we obtained the following results. The material thermomechanical properties used for the simulations are displayed in the first part. The application of the finished differences method with three time steps of the second order, in the case of a constant thermal gradient applied on the microscopic cell is presented in the second part. Finally, the validation of the homogenization computation is presented in the third part.

Material Thermomechanical Properties

We consider a graphite fiber reinforced composite similar to APC2 [7]. Its thermomechanical properties are given below.

Thermal properties of fiber and matrix constituents are given in Table 1. Mechanical properties of fiber and matrix constituents are given in Table 2.

TABLE 1. Thermal Properties

Matrix Thermal Properties	Values
Conductivity k ($\text{W.m}^{-1} \cdot ^\circ\text{C}^{-1}$)	0.3
Expansion coefficient α ($^\circ\text{C}^{-1}$)	50.e-6
Graphite Fibers Thermal Properties	Values
Transverse Conductivity k_t ($\text{W.m}^{-1} \cdot ^\circ\text{C}^{-1}$)	3.0
Longitudinal Conductivity k_f ($\text{W.m}^{-1} \cdot ^\circ\text{C}^{-1}$)	16.0
Transverse Expansion coefficient α_t ($^\circ\text{C}^{-1}$)	10.e-6
Longitudinal Expansion coefficient α_f ($^\circ\text{C}^{-1}$)	-1.e-6

TABLE 2. Mechanical Properties

Matrix Mechanical Properties	Values
Young's modulus E (GPa)	3.6
Shear modulus G (GPa)	1.3
Poisson's ratio ν	0.4
Graphite Fibers Mechanical Properties	Values
Transverse Elastic modulus E_t (GPa)	15.0
Longitudinal Elastic modulus E_f (GPa)	230.0
Shear modulus G_f (GPa)	20.0
Torsion modulus G_t (GPa)	5.0
Poisson's ratio ν_t	0.4
Poisson's ratio ν_{tf}	0.013
Poisson's ratio ν_{ft}	0.25

And for both composite constituents one considers $\rho.C_p = 2.0 \cdot 10^6 \text{ J} \cdot ^\circ\text{C}^{-1} \cdot \text{m}^{-3}$.

Non-Linear Thermal Calculation With Three Time Steps Method

We impose a constant thermal gradient along Y axis on the microscopic cell. Temperature field obtained with three time steps method is calculated and presented on Fig. 4. The three time steps method allows using larger time steps for the non-linear

calculations than with other method. The C.F.L. criterion for the presented configuration is $\Delta t_c \approx 4.10^{-2}$ s, and we used a time step of $\Delta t = 10^{-1}$ s for the computation.

FIGURE 4. Microscopic cell mesh of 4 fibers in a matrix realized with “CNEM” method (on the left). Temperature field obtained with a constant thermal gradient imposed on the microscopic cell (right).

Validation Of The Homogenization Computation

The homogenization computation is validated by realizing elementary tests on the microscopic cell. One applies successively the homogenization method to three elementary fiber geometrical configurations. The volume fraction of fiber used for computations is $2/3$. Homogenized thermomechanical properties are thus calculated.

The results are listed in Table 3 and in Table 4.

TABLE 3. Homogenized Thermomechanical Properties

Homogenized Thermomechanical Properties	Fibers Along X Axis	Fibers Along Y Axis
Constitutive tensor (GPa)	$\begin{bmatrix} 1.5525e5 & 2511.2 & 0 \\ 2511.2 & 8472.6 & 0 \\ 0 & 0 & 11150 \end{bmatrix}$	$\begin{bmatrix} 8472.6 & 2511.2 & 0 \\ 2511.2 & 1.5525e5 & 0 \\ 0 & 0 & 11150 \end{bmatrix}$
Thermal Conductivity tensor (W.m ⁻¹ . °C ⁻¹)	$\begin{bmatrix} 10.767 & 0 \\ 0 & 12.579 \end{bmatrix}$	$\begin{bmatrix} 12.579 & 0 \end{bmatrix}$
Thermal Expansion tensor (°C ⁻¹)	$\begin{bmatrix} -5.663e-7 \\ 2.3525e-5 \\ 0 \end{bmatrix}$	$\begin{bmatrix} 2.3525e-5 \\ -5.663e-7 \\ 0 \end{bmatrix}$

TABLE 4. Homogenized Thermomechanical Properties

Homogenized Thermomechanical Properties	Fibers Along Z Axis
Constitutive tensor (GPa)	$\begin{bmatrix} 9703.3 & 3293.6 & 0 \\ 3293.6 & 9703.3 & 0 \\ 0 & 0 & 2984.3 \end{bmatrix}$

Thermal Conductivity tensor ($\text{W.m}^{-1} \cdot ^\circ\text{C}^{-1}$)

$$\begin{bmatrix} 1.1314 & 0 \\ 0 & 1.1314 \end{bmatrix}$$

Thermal Expansion tensor ($^\circ\text{C}^{-1}$)

$$\begin{bmatrix} 2.0638e-5 \\ 2.0638e-5 \\ 0 \end{bmatrix}$$

One shows that homogenized thermomechanical properties are close to experimental measurements. Therefore the homogenization computation is validated.

CONCLUSION

Residual stress development occurring within the composite during the on-line consolidation process results mainly from two factors : first the thermomechanical properties differences between the composite constituents and secondly the high thermal gradients occurring within the material. The evolution of the material thermomechanical properties must thus be taken into account in the calculation. The multi-scale modeling based on the Constrained Natural Element Method allows taking into account the material properties evolution during the on-line consolidation process. The homogenization computation is validated as usual by realizing elementary tests on the microscopic cell. The prospects for the study are first to realize a global simulation of the industrial process and then to compare the results of the numerical simulation with the industrial experimental results. Secondly, we will introduce a model simulating the solidification front progression within the composite, by using the Level-Set method [8]. This will allow taking into account the crystallization rate evolution of the material which is essential to evaluate the residual stress field within the composite.

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