

Hierarchical Multiscale Process Modeling of a Textile Composite Y-Joint for the Aurora D8 Aircraft

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Abstract. Woven polymer matrix composites (PMCs) are widely used in aerospace applications for their favorable specific properties. However, the behavior of the inter- and intra-tow matrix during manufacturing of woven PMCs is difficult to isolate experimentally due to geometric and processing complexities. Classical closed-form homogenization approaches allow for composite thermo-chemo-mechanical properties to be characterized at any fiber volume fraction. In this work, hierarchical multiscale process modeling is used to apply virtual curing to the inter- and intra-tow matrix materials of a plain weave repeating unit cell (RUC). Thermo-chemo-mechanical property evolution within the tows is calculated using the Concentric Cylinder Model (CCM) and the Rule of Mixtures (ROM). Curing is implemented through user-written subroutines within the commercial finite element method software Abaqus. Virtual curing results are compared with those from a linear-elastic thermal cool down simulation in Abaqus. Results indicate that tow property evolution during curing has a non-negligible effect on the final stress state.

Keywords: process modeling, multiscale, woven PMCs.

1 Introduction

Woven Polymer Matrix Composites (PMCs) are widely considered for use in various aerospace applications due to their superior damage tolerance over traditional unidirectional laminates. However, woven PMCs are still highly susceptible to the growth of residual stresses in the inter- and intra-tow matrix during the curing process. Their complex architecture also influences the final stress state. Due to advancements in high-fidelity computational analysis tools, virtual design and manufacturing optimization of woven PMCs has greatly increased.

Generally, high-fidelity virtual design tools come at a high computational cost. NASA Vision 2040 highlights a demand for robust computational tools, and the development of Integrated Computational Material Engineering (ICME) schemes calls for physics-based models capable of linking length-scales [1]. Process modeling of woven PMCs has been rarely studied in this nature. This technique is crucial to interpret

negligible effects of the curing process and make accurate predictions on end-of-cure stress states [2-6]. A cure-hardening linear-elastic (CHILE) model proposed by Maiarù et al. was used to predict the effects of curing on mechanical performance of PMC microstructures with some consideration toward plain-weave PMCs [7, 8]. Three-dimensional (3D) woven PMCs have been modeled to predict stress concentrations induced by a thermal cool down and compared with micro-cracked areas obtained by micro-computed tomography (micro-CT) [9]. Large differences in coefficients of thermal expansion (CTE) between the tow and matrix material is a driving factor for high residual stresses in the matrix. Process modeling was applied to the inter-tow matrix of a 3D woven PMC repeating unit cell (RUC) using a CHILE approach [10]. Residual stress predictions showed chemical shrinkage and material property evolution to be critical components of the processing, and stress concentrations near the binder tow were comparable to micro-CT data. Boundary condition and cure cycle studies were conducted on a virtually cured 2D woven PMC to determine the effect of the tow architectures and chemical shrinkage [11, 12]. It was concluded that process modeling accounting for chemical shrinkage has a non-negligible effect on the end stress state. However, only the inter-tow matrix properties were allowed to evolve during curing.

This work observes the impact of tow and inter-tow matrix curing on the end-stress state of a plain weave unit cell. Modeling procedures for the 2D woven RUC were maintained from Bukenya et. al. [11]. Virtual curing is applied to the unit cell in a process modeling framework that leverages the commercial FE software suite Abaqus with user-written subroutines. Evolution of tow thermo-chemo-mechanical properties as a function of cure are determined with closed-form homogenization using the Concentric Cylinder Model (CCM) and Rule of Mixtures (ROM) under a hierarchical multiscale process modeling approach. The tow contains AS4 carbon fiber homogenized with RIM R135/H1366 at 80% fiber volume fraction. The inter-tow matrix material consists of RIM R135/H1366. Flat Boundary Conditions (FBCs) are applied in this study as shown in [11]. Preliminary results are compared against a case where only the inter-tow matrix is virtually cured, as well as a linear-elastic thermal cool down in Abaqus modeled with constant room-temperature material properties.

This manuscript is outlined as follows. Section 2 describes the methodology used to develop the computational model. Section 3 discusses the results and infers the optimal boundary condition configuration. Section 4 concludes the current findings and introduces future efforts to expand this work.

2 Introduction

2.1 Theory

Curing of thermosetting polymers results in heat generation and conduction, as well as chemical reactions brought about by changes of phase from liquid to a cross-linked solid structure. The polymer stiffness increases with degree of cure because of the cross-linking networks forming. The result is a buildup of residual stress. The constitutive stress evolution equation using is defined as:

$$\sigma_{ij}(\phi, T) = [C_{ijkl}(\phi, T)] \left[\varepsilon_{kl}^{tot}(\phi, T) - \left(\varepsilon_{kk}^{th}(\phi, T) + \varepsilon_{kk}^c(\phi, T) \right) \delta_{kl} \right] \quad (1)$$

where, ε^{tot} is the total strain, ε^{th} is the thermal strain, and ε^c is the chemical shrinkage strain. C_{ijkl} is the six-by-six instantaneous stiffness matrix at degree of cure ϕ and temperature T containing isotropic mechanical properties for the polymer matrix during cure:

$$C_{ij}(\phi, T) = \frac{E(\phi, T)}{[1 + \nu(\phi, T)][1 - 2\nu(\phi, T)]} * \dots \quad (2)$$

$$\begin{bmatrix} 1 - \nu(\phi, T) & \nu(\phi, T) & \nu(\phi, T) & 0 & 0 & 0 \\ \nu(\phi, T) & 1 - \nu(\phi, T) & \nu(\phi, T) & 0 & 0 & 0 \\ \nu(\phi, T) & \nu(\phi, T) & 1 - \nu(\phi, T) & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 - 2\nu(\phi, T) & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 - 2\nu(\phi, T) & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 - 2\nu(\phi, T) \end{bmatrix}$$

where $E(\phi, T)$ and $\nu(\phi, T)$ are the temperature- and cure-dependent Young's Modulus and Poisson's Ratio, respectively.

The transient heat transfer equation considers the conduction and nonlinear internal heat generation of the polymer matrix during cure:

$$\rho c_p \frac{\partial T}{\partial t} = k_x \frac{\partial^2 T}{\partial x^2} + k_y \frac{\partial^2 T}{\partial y^2} + k_z \frac{\partial^2 T}{\partial z^2} + \frac{\partial H}{\partial t} \quad (3)$$

where ρ , c_p , and T are the density, specific heat, and temperature. The term H represents the internal enthalpic heat source. Thermal conductivities k are subscripted to represent an anisotropic material in the x -, y -, and z -directions. The material system for the RUC used in this study is transversely isotropic, and therefore $k_y = k_z$. Derivations for the kinetic model used in this study are given by Bukenya et. al. [12].

2.2 Closed-Form Homogenization

To predict the effective composite properties for the tow during curing, constant properties of AS4 carbon fiber were homogenized with cure- and temperature-dependent properties of RIM R135/H1366 at 80% fiber volume fraction. Composite thermal properties were estimated using the rule of mixtures (ROM) as described in [13], while elastic properties were homogenized using the concentric cylinder model (CCM) as outlined in [14]. Thermo-chemo-mechanical property evolution for the RIM system are provided by Shah et. al. [15], while the fully cured properties are detailed in Table 1. AS4 carbon fiber properties are given in Table 2.

Table 1. Thermo-chemo-mechanical properties for RIM R135/H1366.

Property		Value	Unit
Young's Modulus	E	2.50	GPa
Poisson's Ratio	ν	0.37	-
Coefficient of Thermal Expansion (CTE)	α	70	$10^{-6}/^{\circ}\text{C}$
Thermal Conductivity	k	0.245	$\text{mW}/(\text{mm} \cdot ^{\circ}\text{C})$
Specific Heat Capacity	c_p	1.60E+09	$\text{mJ}/(\text{tonnes} \cdot ^{\circ}\text{C})$
Density	ρ	1.20E-09	$\text{tonnes}/\text{mm}^3$
Cure Temperature	T_{cure}	80	$^{\circ}\text{C}$
Room Temperature	T_{room}	20	$^{\circ}\text{C}$
Cure Time	t_{cure}	10200	s
Gel Point	ϕ_{gel}	0.82	-

Table 2. Constant thermomechanical properties for AS4 carbon fiber.

Property		Value	Unit
Longitudinal Young's Modulus	E_{11}	231	GPa
Transverse Young's Modulus	$E_{22} = E_{33}$	15	GPa
In-Plane Poisson's Ratio	$\nu_{12} = \nu_{13}$	0.21	-
Out-of-plane Poisson's Ratio	ν_{23}	0.30	-
In-Plane Shear Modulus	$G_{12} = G_{13}$	15.8	GPa
Longitudinal Coefficient of Thermal Expansion (CTE)	α_{11}	-0.50	$10^{-6}/^{\circ}\text{C}$
Transverse Coefficient of Thermal Expansion (CTE)	$\alpha_{22} = \alpha_{33}$	15	$10^{-6}/^{\circ}\text{C}$
Longitudinal Thermal Conductivity	k_{11}	6.83	$\text{mW}/(\text{mm} \cdot ^{\circ}\text{C})$
Transverse Thermal Conductivity	$k_{22} = k_{33}$	0.1366	$\text{mW}/(\text{mm} \cdot ^{\circ}\text{C})$
Specific Heat Capacity	c_p	1.13E+09	$\text{mJ}/(\text{tonnes} \cdot ^{\circ}\text{C})$
Density	ρ	1.79E-09	$\text{tonnes}/\text{mm}^3$

2.3 Cure Cycle

The cure cycle used in this study is shown in Fig. 1. The temperature profile depicted in this plot is consistent with that used in previous studies [11]. The corresponding degree of cure evolution was calculated from the kinetic model used in [12].

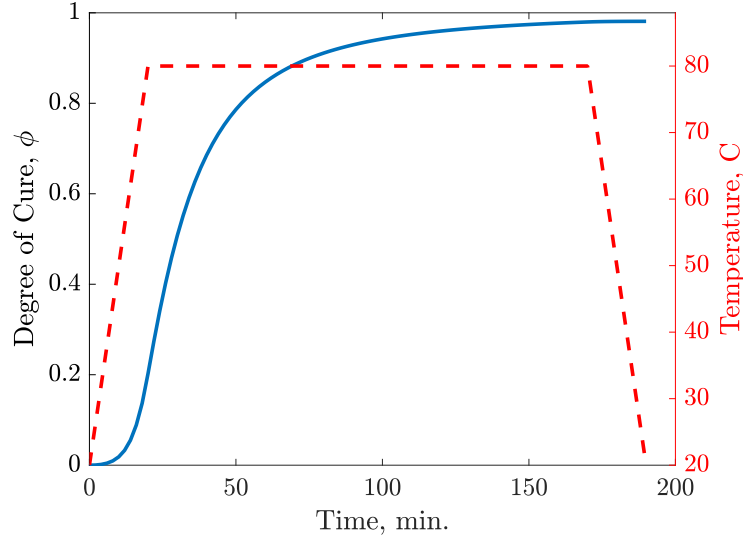


Fig. 1. Temperature profile and degree of cure with respect to curing time.

2.4 Case Study

Three cases were observed to determine the impact of tow property evolution on the final residual stress of the 2D woven PMC. The first case involved virtual manufacturing of both the tow and inter-tow matrix materials using the cure cycle in Fig. 1. In the second case, virtual curing was applied only to the inter-tow matrix. The tow properties were homogenized with end-of-cure constituent properties and held constant during curing. The final case assumed a linear elastic thermal cool down with constant properties at room temperature. These case studies are tabulated below in Table 3.

Table 3. Case study to determine the contribution of intra-tow matrix curing on residual stress predictions.

Case Number	Analysis
1	Tow and Inter-Tow Matrix Curing
2	Inter-Tow Matrix Curing Only
3	End-of-Cure Properties and Thermal Cool Down

3 Results and Discussion

Results from this study are shown below in Fig. 2 with the inter-tow matrix isolated.

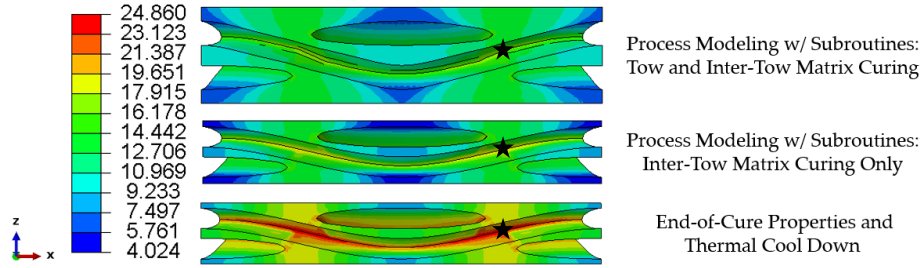


Fig. 2. Residual stress concentrations in the inter-tow matrix sliced at mid-width along y-direction; residual stress induced by process modeling with (top) and without (middle) tow curing, and a linear-elastic thermal cool down (bottom). Maximum principal stress magnitudes given in MPa. Star icon indicates a point of interest.

From Fig. 2, the stresses in the RUC are not homogenous. Areas of high stress are concentrated at the interface between the tows and matrix. This non-uniform distribution indicates potential weak points that could affect the overall mechanical performance of the composite material. The high-stress regions suggest that these interfaces are more likely to experience damage or failure, which could propagate through the material, compromising its structural integrity. With process modeling, the influence of various processing parameters and material properties on the stress concentrations can be identified. Additionally, this insight can guide the development of more accurate predictive models for composite behavior, ensuring that simulations closely match real-world performance.

To further investigate this, a point of interest (see Fig. 2) in the inter-tow matrix material at an area of high stress was selected and plotted across each case. This stress evolution is shown below in Fig. 3.

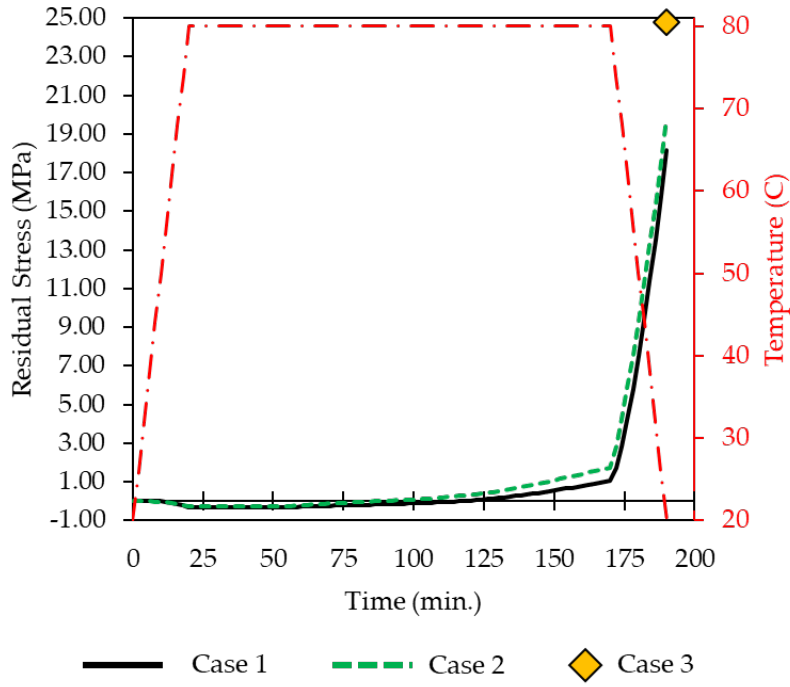


Fig. 3. Residual stress evolution for Case 1, Case 2, and Case 3.

Fig. 3 shows that between Cases 1 and 2, the stress begins to largely deviate at approximately $t = 100$ minutes. Case 2 also yields a higher stress state than Case 1. This is because the tows in Case 2 were homogenized with end-of-cure matrix properties, where the stiffness is maximized, and held constant during curing. The tows in Case 1 were homogenized as a function of the cure, and thus were subjected to evolving matrix stiffness. Constant end-of-cure properties used in Case 3 yielded an end stress state even higher than Case 2, emphasizing a critical need for process modeling to predict thermo-mechanical property evolution during curing. This distinction between the three cases highlights the impact of matrix stiffness evolution on residual stress development. In Case 3, the assumption of constant high stiffness throughout the curing process led to higher stress predictions. This suggests that failing to account for matrix property evolution can result in overly conservative estimates of residual stress which may not appropriately reflect the behavior of woven PMCs. In contrast, Case 1 incorporates the assumption that stiffness evolves as a function of cure and temperature, leading to a more accurate representation of the end stress state under these processing conditions. These results imply that modeling practices similar to Case 3 may overestimate the final

stress state highlight the need for more refined modeling approaches to prevent excessively cautious predictions.

The final maximum principal stress value at the area of interest is shown in Table 4 for each case. The relative percent difference was calculated with respect to Case 1.

Table 4. Comparison of final (maximum principal) stress states and relative percent difference with respect to Case 1.

Case Number	Analysis	Final Stress (MPa)	Percent Difference (Relative to Case 1)
1	Tow and Inter-Tow Matrix Curing	18.15	–
2	Inter-Tow Matrix Curing Only	19.84	+ 9.31 %
3	End-of-Cure Properties and Thermal Cool Down	24.76	+ 36.42 %

It can be clearly seen from Table 4 that restricting material property evolution to only the inter-tow matrix overestimates the final stress in the matrix relative to Case 1 by 9.31%. However, a simplified thermal cool down with room temperature properties overpredicts the final stress by 36.42%. This significant overestimation in Case 3 underscores the limitations of a simplified linear-elastic model that does not account for the dynamic nature of the curing process. The use of end-of-cure properties and a linear-elastic thermal cool down assumes a constant material state, and thus fails to capture the cure-dependent changes in matrix stiffness and the resultant stress distribution accurately. As a result, the predicted stress is much higher than in more refined constitutive laws, such as the CHILE model used in Cases 1 and 2. The 9.31% overestimation in Case 2 indicates that while focusing only on the inter-tow matrix provides a closer approximation than a fully simplified model, it still does not accurately reflect the complex interplay between the tows and matrix during curing. This suggests that including the evolving properties of both the tow and inter-tow matrix, as in Case 1, is crucial for obtaining a more realistic stress profile. Furthermore, the relative differences provide insight into the sensitivity of the final stress state to different modeling assumptions. This sensitivity analysis can guide future research focus toward improving models to better capture the material behavior during curing.

4 Conclusions

The work presented in this study demonstrates that the stress prediction in woven PMCs significantly depends on the modeling approach. Virtual manufacturing was applied to both the tow and matrix material of a 2D woven unit cell. A closed-form homogenization approach was utilized to approximate composite properties as a function of cure. Results show that when tow property evolution is not included, the end stress state is overestimated by nearly 10%. Furthermore, a linear-elastic thermal cool down with fully cured properties will overestimate the residual stress in a 2D woven PMC. Findings from this study emphasize the importance of incorporating detailed material

behavior into computational models for composite manufacturing, aligning with ICME principles. Simplified approaches can lead to significant errors in stress prediction, potentially resulting in suboptimal design and reduced performance in practical applications. Comprehensive process models that predict evolving material properties during curing provide the most accurate stress predictions, thereby enhancing the reliability and performance of aerospace components. Hierarchical multiscale process modeling, leveraged within an ICME framework, empowers engineers to achieve more accurate simulations, leading to better-informed decisions in the design and manufacturing processes.

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