

Process Modeling of Woven Textiles

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Woven polymer matrix composites offer numerous advantages over traditional unidirectional laminates. Processing conditions affect residual stress that builds up during manufacturing. This work proposes the analysis of three curing parameters on the local residual stress distribution of a plain weave textile architecture, including chemical shrinkage, the temperature cool down, and the evolution of matrix properties as a function of curing. Virtual curing is applied to the inter-tow matrix material of the plain weave Repeating Unit Cell (RUC) modeled in TexGen. Curing is implemented through user-written subroutines within the commercial software suite Abaqus. Results from process modeling are compared with a linear-elastic thermal cool down in Abaqus. A boundary conditions study is also conducted to compare the residual stress build up predicted by Flat (FBCs) and Periodic Boundary Conditions (PBCs). Preliminary results indicate that a thermal cool down overestimates the end-of-cure stresses in the matrix. Process modeling is conducted with and without chemical shrinkage, then compared with a thermal cool down. Results show that 11.32% of the final stress state is due to chemical shrinkage. Material property evolution during curing also has a non-negligible effect on the end stress.

I. Introduction

Woven Polymer Matrix Composites (PMCs) are widely considered for use in various aerospace applications due to their superior in-plane specific properties over traditional unidirectional laminates. However, woven PMCs are still highly susceptible to 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-woven 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

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was applied to the inter-tow matrix of a 3D woven PMC 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 influences on computational homogenization of periodic woven structures have been studied [11-12]. Efforts must be made to reduce inherent computational expenses. Therefore, the influence of boundary conditions on process-induced stress evolution within woven PMCs must be studied. Understanding this impact provides insight when building accurate and computationally robust physics-based models. Furthermore, chemical shrinkage evolution is rarely accounted for when studying residual stress build up in woven textiles. The impact of these two curing mechanisms must be understood to accurately quantify the end stress state of woven textiles.

The objective of this study is to determine the effects of process modeling on the buildup of residual stresses within a woven PMC repeating unit cell (RUC). A secondary objective is to quantify the effect of chemical shrinkage evolution on the end stress state of the woven PMC. A two-dimensional (2D) woven PMC was chosen to reduce the geometric complexity. RIM R135/H1366 epoxy was chosen as the resin system for this study. The tows are AS4 carbon fiber coupled with RIM R135/H1366 at 80% fiber volume fraction modeled with the open-source software TexGen. Process modeling is performed on the inter-tow matrix material with user-written Fortran subroutines within the finite element (FE) commercial software Abaqus. A linear-elastic thermal cool down in Abaqus is then conducted using constant properties at room temperature. Preliminary end-of-cure stress results from process modeling and the thermal cool down are compared. A boundary condition study is conducted using Flat (FBCs) and Periodic (PBCs) Boundary Conditions to further develop an accurate and computationally efficient model. From this study, an optimal BC configuration is chosen. The effect of chemical shrinkage and on the final stress state are then quantified.

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

II. Methodology

Process modeling leverages robust computational analysis tools and software to allow for high-fidelity virtual design, testing, and optimization of woven PMCs. It accounts for evolution of material properties as a function of the degree of cure and chemical shrinkage in the matrix. Thus, accurate stress-strain response can be predicted for a wide variety of material systems and cure cycles when process modeling is integrated into woven PMC design and analysis. The constitutive law, governing heat equation, and cure kinetics used in this study are outlined in Section II.A. The procedure used to produce create the woven PMC RUC is discussed in Section II.B. The boundary conditions (BCs) study is defined with FBC and PBC equations given in Section II.C.

A. 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:

$$\sigma_i(t) = [C_{ij}(t)] \left[\varepsilon_j^t(t) - \left(\varepsilon_j^{th}(t) + \varepsilon_j^c(t) \right) \right] \quad (1)$$

where, ε^t is the total strain, ε^{th} is the thermal strain, and ε^c is the chemical shrinkage strain. C_{ij} is the six-by-six instantaneous stiffness matrix at time t containing isotropic mechanical properties for the polymer matrix during cure:

$$C_{ij}(t) = \frac{E(t)}{(1 + \nu(t))(1 - 2\nu(t))} \begin{bmatrix} 1 - \nu(t) & \nu(t) & \nu(t) & 0 & 0 & 0 \\ \nu(t) & 1 - \nu(t) & \nu(t) & 0 & 0 & 0 \\ \nu(t) & \nu(t) & 1 - \nu(t) & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 - 2\nu(t) & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 - 2\nu(t) & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 - 2\nu(t) \end{bmatrix} \quad (2)$$

where $E(t)$ and $\nu(t)$ are the time-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 $k_y = k_z$.

A relationship can be made between the rate of heat flow $\frac{\partial H}{\partial t}$ and the rate of reaction $\frac{d\phi}{dt}$:

$$\frac{d\phi}{dt} = \frac{1}{H_T} \frac{dH}{dt} \quad (4)$$

where H_T is the total heat of reaction at the end of curing. The degree of cure ϕ of the matrix is the integral of Eq. (4) with respect to time t :

$$\phi(t) = \frac{1}{H_T} \int_0^t \frac{dH}{dt} dt = \frac{H_{pr}}{H_T} \quad (5)$$

where H_{pr} is the partial heat dissipated at a given time t . The rate of cure can be expressed mathematically as a function of temperature and degree of cure:

$$\frac{d\phi}{dt} = f(T, \phi), \quad f(T, \phi) \geq 0 \quad (6)$$

This function is in turn defined with a semi-empirical expression proposed by Kamal [13] and uses Arrhenius temperature-dependent terms to assign a direct relation between the rate of reaction and degree of cure:

$$\frac{d\phi}{dt} = (K_1 + K_2 \phi^m)(1 - \phi^n) \quad (7)$$

where K_1 and K_2 are the Arrhenius rate reactions with curve-fitted exponent constants m and n . The reaction rates introduce frequency-like constants A_1 and A_2 and with activation energies ΔE_{a1} and ΔE_{a2} as a function of absolute temperature T :

$$K_i = A_i \exp\left(-\frac{\Delta E_{ai}}{RT}\right) \quad i = 1, 2 \quad (8)$$

where R is the universal gas constant $8.3145 \frac{\text{J}}{\text{mol}\cdot\text{K}}$. The RIM R135/H1366 resin system used in this study was characterized in-house at the University of Massachusetts Lowell [14]. The Prout-Thompkins model was used for simplicity and under isothermal conditions, where $A_2 = \Delta E_{a2} = 0$ [7].

The cure cycle used in this study is shown in Figure 1. The cure kinetics constants are listed in Table 1. Additionally, the thermomechanical material properties for RIM R135/H1366 polymer matrix and AS4/RIM R135/H1366 tows are given in Table 2 and Table 3, respectively.

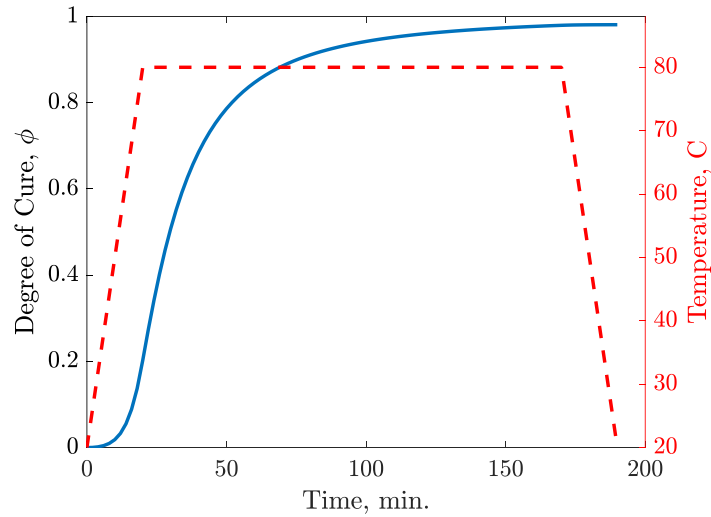


Fig. 1 Temperature profile and degree of cure with respect to curing time.

Table 1 Cure Kinetics Constants for RIM R135/H1366

Property		Unit	Value
Exponents	m	[-]	0.3
	n	[-]	1.5
Rate Constant	A_1	[sec ⁻¹]	11000
Activation Energy	ΔE_{a1}	[kJ/mol]	46.7

Table 2 Thermo-chemo-mechanical Properties for RIM R135/H1366

Property	Unit	Value
E	2.50	[GPa]
ν	0.37	[-]
α	70	[10 ⁻⁶ /°C]
k	0.245	$\left[\frac{\text{mW}}{\text{mm} \cdot ^\circ\text{C}} \right]$
c_p	1.60E+09	$\left[\frac{\text{mJ}}{10^3 \text{kg} \cdot ^\circ\text{C}} \right]$
ρ	1.20E-09	$\left[\frac{10^3 \text{kg}}{\text{mm}^3} \right]$
T_{cure}	80	[°C]
T_{Room}	20	[°C]
t_{cure}	10200	[s]
ϕ_{gel}	0.82	[-]

Table 3 Thermomechanical Properties for AS4/RIM R135/H1366 Tow with 80% Fiber Volume Fraction

Property	Value	Unit
E_A	185.3	[GPa]
E_T	10.74	[GPa]
ν_{12}	0.242	[-]
ν_{23}	0.3984	[-]
G_{12}	6.93	[GPa]
G_{23}	3.84	[GPa]
α_A	-0.334	[10 ⁻⁶ /°C]
α_T	27.82	[10 ⁻⁶ /°C]
k_A	5.5130	$\left[\frac{\text{mW}}{\text{mm} \cdot ^\circ\text{C}} \right]$

k_T	0.1556	$\left[\frac{\text{mW}}{\text{mm} \cdot ^\circ\text{C}} \right]$
c_p	1.1978E+09	$\left[\frac{\text{mJ}}{10^3 \text{kg} \cdot ^\circ\text{C}} \right]$
ρ	1.6720E-09	$\left[\frac{10^3 \text{kg}}{\text{mm}^3} \right]$

B. Modeling

The geometry used in this study is shown in Figure 2. The tow volume fraction of the unit cell is 0.80. The in-plane width and out-of-plane thickness are 2.6 mm and 0.4 mm, respectively [8]. The tow geometry was created via Python scripting in the open-source software TexGen. The IGES file containing the tows was then imported into Abaqus/CAE and used to construct the matrix domain. The tows and matrix domain were then merged to apply discrete material orientations, material properties, and boundary conditions.

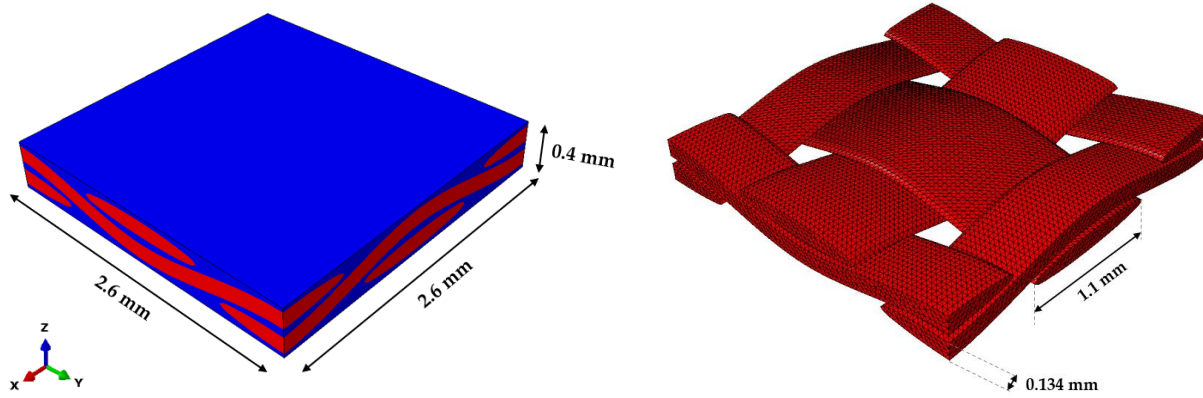


Fig. 2 Schematic of 2D woven PMC displays the full RUC with matrix shown in blue and tows shown in red (left); the constituent tows with dimensions (right). The XYZ triad indicates the global reference frame.

The unit cell was meshed with 280,586 quadratic tetrahedral temperature-displacement elements (C3D10T). A periodic mesh was generated on the RUC with the procedure outlined in Jendrysik et al [15].

C. Boundary Conditions

The boundary condition (BC) study consists of two sets of BCs applied to the RUC during curing. Flat boundary conditions (FBCs) and Periodic (PBCs) are proposed to simulate the effect material surrounding the RUC. However, FBCs imply that the faces of the RUC remain flat while PBCs enforce periodic deformation. Consider an undeformed cuboid RUC with a corner point origin (0,0,0). The cuboid possesses dimensions L_1 , L_2 , and L_3 along directions x_1 , x_2 , and x_3 .

The equations corresponding to the PBCs are:

$$\begin{aligned}
 u_1(L_1, x_2, x_3) - u_1(0, x_2, x_3) &= \varepsilon_{11} L_1 \\
 u_2(L_1, x_2, x_3) - u_2(0, x_2, x_3) &= 2\varepsilon_{12} L_1 \\
 u_3(L_1, x_2, x_3) - u_3(0, x_2, x_3) &= 2\varepsilon_{13} L_1 \\
 u_1(x_1, L_2, x_3) - u_1(x_1, 0, x_3) &= 2\varepsilon_{21} L_2 \\
 u_2(x_1, L_2, x_3) - u_2(x_1, 0, x_3) &= \varepsilon_{22} L_2 \\
 u_3(x_1, L_2, x_3) - u_3(x_1, 0, x_3) &= 2\varepsilon_{23} L_2 \\
 u_1(x_1, x_2, L_3) - u_1(x_1, x_2, 0) &= 2\varepsilon_{31} L_3 \\
 u_2(x_1, x_2, L_3) - u_2(x_1, x_2, 0) &= 2\varepsilon_{32} L_3 \\
 u_3(x_1, x_2, L_3) - u_3(x_1, x_2, 0) &= \varepsilon_{33} L_3
 \end{aligned} \tag{9}$$

where u_1 , u_2 , and u_3 represent displacements of the RUC along directions x_1 , x_2 , and x_3 respectively, and ε_{ij} are tensorial strains. PBCs are applied in Abaqus with the *EQUATION key to pair nodes on opposite faces of the RUC.

FBCs are applied with the same Abaqus key using reference points RPX, RPY, and RPZ located at $(L_1, 0, 0)$, $(0, L_2, 0)$, and $(0, 0, L_3)$, respectively. The L_1 (Right), L_2 (Top), and L_3 (Front) faces are then paired with their corresponding reference points to enforce uniform and parallel displacement during expansion and contraction. For a given mesh size, FBCs are computationally efficient than PBCs.

The equations corresponding to the FBCs are:

$$\begin{aligned} u_1^{Right} - u_1^{RPX} &= 0 \\ u_2^{Top} - u_2^{RPY} &= 0 \\ u_3^{Front} - u_3^{RPZ} &= 0 \end{aligned} \quad (10)$$

D. Chemical Shrinkage Effects

Three cases were observed to determine the effects of chemical shrinkage evolution on the final residual stress of the 2D woven PMC. The first case used process modeling to determine the effect of the full cure cycle on the final stress. The second case isolated the effect of chemical shrinkage. The final case assumed a linear elastic thermal cool down with constant properties at room temperature. This case study is tabulated below in Table 4.

Table 4 Case Study to Determine the Contribution of Matrix Shrinkage and Evolution of Matrix Thermomechanical Properties on Residual Stress Prediction

Case Number	Analysis
1	Evolution of Thermomechanical Properties with Curing, and Shrinkage
2	Evolution of Thermomechanical Properties with Curing, no Shrinkage
3	Properties at the End of Cure and Thermal Cool Down

III. Results and Discussion

The RUC shown in Figure 2 was subjected to the cure cycle shown in Figure 1. The temperature profile was applied to the $(x_1, x_2, 0)$ and (x_1, x_2, L_3) faces of the RUC. Process modeling is applied only to the matrix material and the tows remain linear-elastic (constant) properties during curing. Section III.A introduces the preliminary results of this study. Section III.B further interprets the results and discusses the selection of boundary conditions.

A. Boundary Condition Effects

At end-of-cure, the residual stress in the matrix is shown for both boundary condition sets using maximum principal stress values in MPa. Figure 3 compares the final residual stress state induced by process modeling and a linear-elastic thermal cool down performed in Abaqus. Mid-width slices along the y-direction were taken to display the inter-tow matrix stress concentrations. The thermal cool down replicated the final stage of the curing cycle shown in Figure 1 using constant matrix and tow properties at room temperature. A deformation scaling factor of 10 was used to observe the stress contours. For both sets of boundary conditions, the Abaqus thermal cool down produced higher residual stress concentrations in this region. This is because a simple thermal cool down fails to account of evolution of material properties as a function of the curing. Stiffness and CTE components are maximum at the end of curing. Furthermore, the final degree of cure for a given resin system is dependent on the curing cycle. The cure cycle used in this study reaches a degree of cure of 0.98. Thus, the matrix is still curing and shrinking during the thermal cool down phase. Process modeling captures this thermochemical evolution of material properties and indicates that the cure cycle can be manipulated to mitigate residual stresses in a woven PMC.

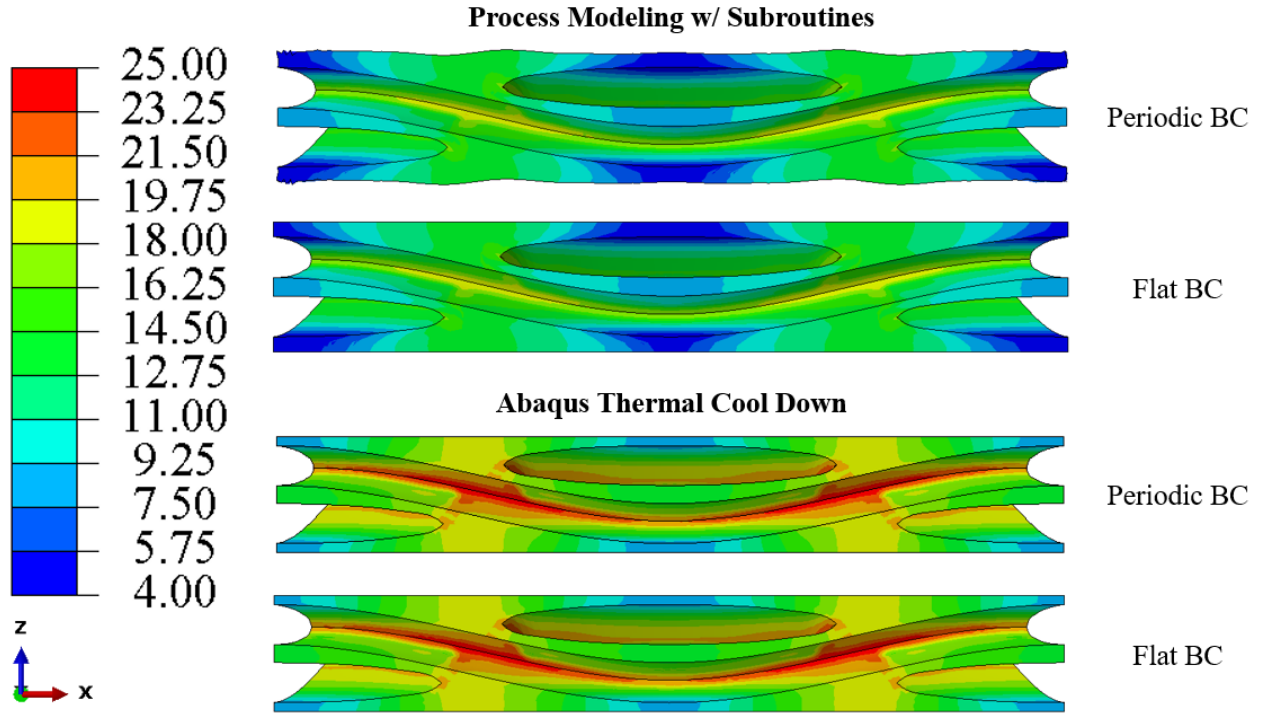


Fig. 3 Residual stress concentrations in the matrix sliced at mid-width along y-direction; residual stress induced by process modeling and a linear-elastic thermal cool down using Periodic BCs and Flat BCs. Maximum principal stress magnitudes given in MPa.

B. Boundary Condition Selection

A matrix element containing high residual stress was chosen and the maximum principal stress was plotted with respect to time t for both sets of boundary conditions.

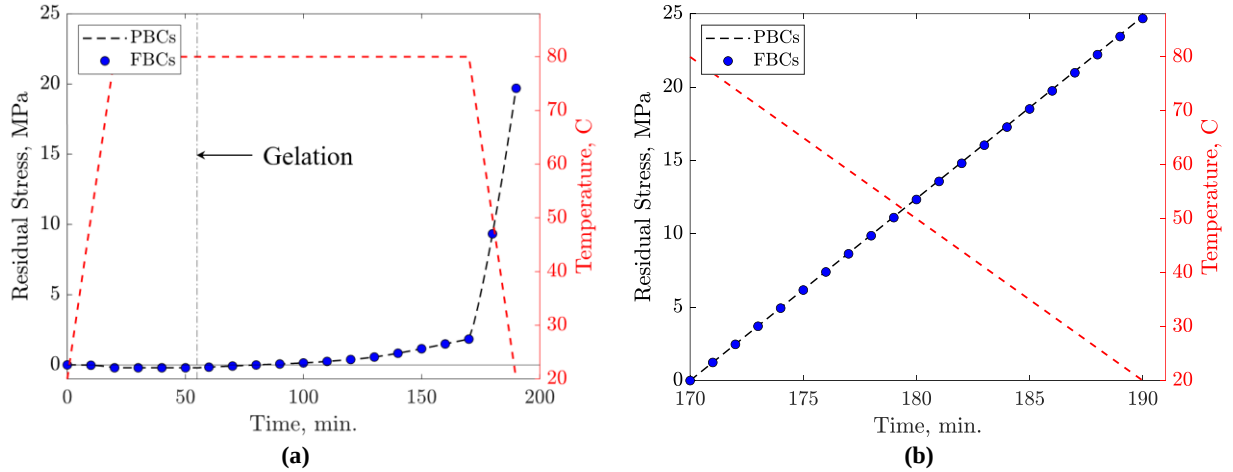


Fig. 4 Periodic Boundary Conditions (PBCs) compared with Flat Boundary Conditions (FBCs) for: (a) process modeling with user-written subroutines and (b) a linear-elastic thermal cool down in Abaqus.

Similar to the comparative stress contours, the plotted element residual stresses show good agreement between FBCs and PBCs. PBCs increased computational time by approximately 47%. Therefore, FBCs are suggested for this model configuration in future studies.

A closer look at Figure 4(a) shows an initial compressive stress in the matrix due to the differences in CTE between tow and matrix material. Moreover, CTE in the matrix is maximized prior to gelation ($\phi_{gel} = 0.82$). Gelation occurs

during the isothermal phase of this cure cycle at approximately $t = 55$ minutes during which the matrix is chemically shrinking. The linear-elastic tow material resists further shrinkage along the fiber direction, and the result is an increase in tensile stress within the matrix. During the cool down phase, the matrix is still shrinking as the degree of cure approaches 1. The stiffness is also evolving with respect to temperature. It is worth noting that this cure cycle did not produce a significant exothermic reaction in the matrix due to the low volume of inter-tow matrix material in the RUC and the high fiber volume fraction in the tows. Thus, no additional heat was generated during cure.

The final maximum principal stress magnitudes are compared between process modeling and an Abaqus thermal cool down in Table 5. The Abaqus thermal cool down accounts for neither thermal nor chemical evolutions in the material. Generally, room temperature values are assumed during a thermal cool down analysis. When compared with a process modeling cure cycle that induces a small exotherm, the higher thermomechanical properties assumed in the thermal cool down dominate at the end of cure.

Table 5 BC Study: Final Stress States between Process Modeling and a Thermal Cool Down in MPa

BC Configuration	Process Modeling with Subroutines	Abaqus Thermal Cool Down
Flat BC	19.64	24.25
Periodic BC	19.70	24.38

C. Impact of Chemical Shrinkage Evolution on Final Stress State

In Figure 5, inter-tow matrix residual stress states are shown using the maximum principal stress distribution for each case in Table 4. The deformation scaling factor was maintained from the boundary condition study, and the scale is in MPa.

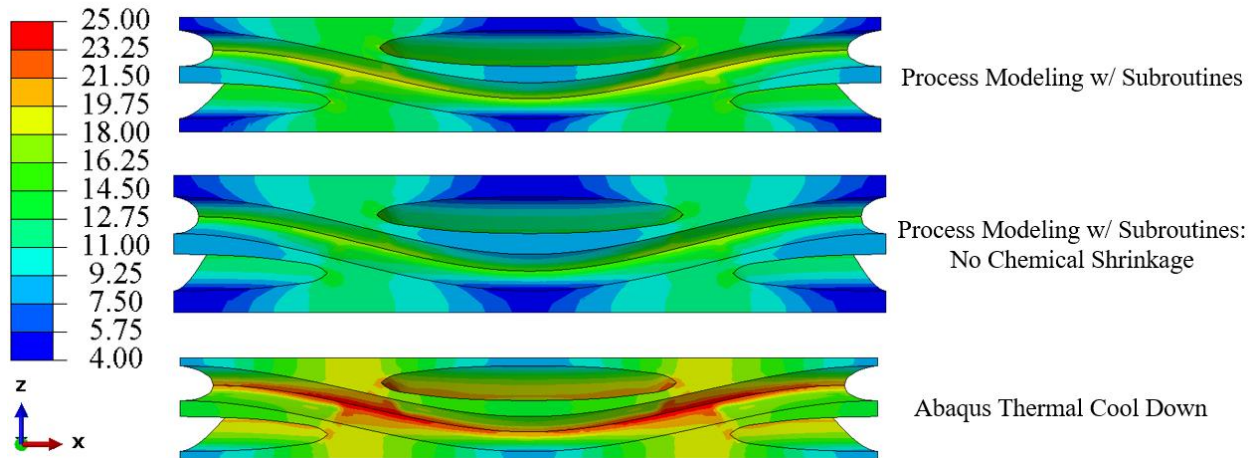


Fig. 5 Residual stress concentrations in the matrix sliced at mid-width along y-direction; residual stress induced by process modeling with and without chemical shrinkage, and a linear-elastic thermal cool down. Maximum principal stress magnitudes given in MPa.

Figure 5 shows a clear difference in final stress states between the two process modeling cases. Disregarding chemical shrinkage results in a lower end stress state. The Abaqus thermal cool down still yielded the highest stress state because stiffness and CTE components were constant and assumed at room temperature.

The residual stress evolution for Cases 1-3 (see Table 4) are shown in Figure 6. As the Abaqus thermal cool down produced a linear relationship between residual stress and time, only the final stress value is plotted.

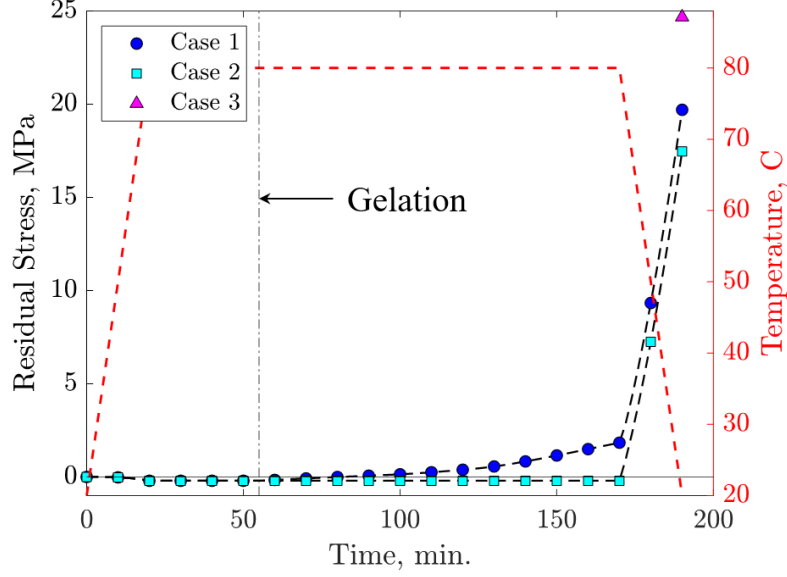


Fig. 6 Residual stress evolution for Case 1, Case 2, and Case 3 (see Table 4).

It can be seen from Figure 6 that neglecting chemical shrinkage (Case 2) results in an underpredicted final stress state. Post-gelation, there is a noticeable increase in stress due to chemical shrinkage (Case 1). Additional non-negligible effects include stiffness and CTE evolution during curing. Without shrinkage, the matrix remains in a state of compression until the cool down phase is initiated. Table 6 shows the final stress states between Cases 1-3 and the percent difference relative to Case 1.

Table 6 Case Study: Comparison of Final (Maximum Principal) Stress States and Relative Percent Error

Case Number	Final Stress (MPa)	Percent Difference (Relative to Case 1)
1	19.64	—
2	17.47	- 11.32 %
3	24.25	+ 25.28 %

Chemical shrinkage accounts for 11.32% of the final stress state. A thermal cool down with room temperature properties overpredicted the final stress by 25.28%. Because process modeling can account for chemical shrinkage, its impact on the final residual stress state can be isolated and quantified.

IV. Conclusions and Future Work

This manuscript has addressed the need to integrate high-fidelity process modeling computational tools for woven composites engineering. The boundary condition study conducted with FBCs and PBCs yielded similar results with a 47% decrease in computational efficiency when PBCs were applied. The effects of process modeling on the residual stress buildup within the inter-tow matrix of a woven PMC unit cell have been presented. It is seen that the curing has a non-negligible influence on the final stress state beyond differences in CTE. This is due to the cure-dependent stiffness properties and shrinkage strains. Results presented in this manuscript imply that the cure cycle can be tailored by modifying the cure cycle parameters to avoid severe increases in residual stress during cure. Comparisons were made between process modeling and an Abaqus thermal cool down. Results imply that neglecting the effect of the evolution of the matrix thermomechanical properties and resin shrinkage during curing leads to an over-estimation of the final residual stress state. Results show that chemical shrinkage accounts for 11.32% of the final stress state. Stiffness and CTE evolution have a significant impact on the state of residual stress. Process modeling allows for curing mechanisms such as chemical shrinkage to be isolated such that their influences can be quantified. In doing so, the final residual stress state in woven PMCs can be tuned. The present work focused on the analysis of the curing

cycle on the textile matrix and neglected the effect of curing on the intra-tow matrix material. Future work will include process modeling applied to both the tow and matrix material to accurately represent dry-fiber tows infused with epoxy resin prior to curing.

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