An analytical tool for studying the impact of process parameters on the mechanical response of composites

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Abstract. The present work presents a numerical framework able to predict the impact of the manufacturing process on the mechanical performance of the composite component. A simple onedimensional thermochemical model has been used to predict the evolution of the degree of cure of the resin for a given thermal cycle. The homogenized properties at the lamina level have been obtained through a classical mixtures law and employed to predict the process-induced deformations. A refined one-dimensional model, derived in the framework of the Carrera Unified Formulation, has been used to provide accurate results with reduced computational costs. The virtual manufacturing framework has been used to investigate the impact of the process parameters on process-induced defects of a simple composite part. Different curing cycles have been considered and their outcomes discussed. The results demonstrate the capability of the present numerical tool to correlate the manufacturing process parameters with the mechanical performances of the final component.

Introduction

Composite materials are increasingly being used in various applications in industry due to their superior mechanical properties [1]. The manufacturing of composite structures for aerospace applications must meet strict requirements in terms of process-induced defects. The use of inautoclave processes ensures higher mechanical performances of the final component by reducing the presence of voids but, on the other hand, involves the use of high temperature and pressure that can lead to residual deformations and stresses. [2]. The process-induced defects may lead to an early failure of the component or to geometrical inaccuracies that make the structural assembly complicated. Numerical tools based on the finite element method (FEM) can be used to predict process-induced defects but, the three-dimensional nature of the problem requires solid models to be used with a consequent high computational cost. In this work, a refined one-dimensional model, developed within the field of Carrera Unified Formulation (CUF) [3], is used to obtain residual deformations due to the curing process accurately with low computational cost [4]. A one-dimensional thermochemical model is used to predict the evolution of temperature and degree of cure during the process of the composite structure [5]. The mechanical properties of the composite laminate are obtained from a micromechanical model based on the law of mixtures [6].

Equations and model

The cure model is based on the heat transfer governing equation through thickness, i.e., the onedimensional Fourier thermal conduction equation:

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$$\dot{Q} + k \frac{\partial^2 T}{\partial z^2} = \rho H_r V_r \frac{d\alpha}{dt} + k \frac{\partial^2 T}{\partial z^2} = \rho c_p \frac{\partial T}{\partial t} \qquad \text{for } T(z,t) \text{ in } (0 < z < l)$$
(1)

where k, ρ , and c_p are the thermal conductivity, density, and specific heat of the composite, respectively, and are assumed constant during the process. α is the degree of cure, H_r is the total heat released from the resin reaction, V_r is the volume fraction of the resin. The thickness of the laminate is equal to *l*. *T* and *t* are temperature and time. The normal to the inplane dimension of the composite is the z-direction. The term \dot{Q} represents the internal heat generated by the exothermic chemical reaction of the resin.

The cure rate for graphite/epoxy material follows this expression, where k_1 , k_2 and k_3 are defined by the Arrhenius equation [5]:

$$\frac{d\alpha}{dt} = (k_1 + k_2 \alpha)(1 - \alpha)(0.47 - \alpha) \quad \text{for } (\alpha \le 0.3)$$

$$\frac{d\alpha}{dt} = k_3(1 - \alpha) \quad \text{for } (\alpha > 0.3)$$

$$k_i = A_i e^{\frac{-\Delta E_i}{RT}} \quad \text{for } i = 1, 2, 3$$
(2)

R is the universal gas constant, A_i are the pre-exponential coefficients, and ΔE_i are the activation energies.

The mechanical properties of the resin are strongly dependent on the curing process. The instantaneous modulus of the resin can be expressed as a function of the degree of cure according to the α mixing rule [6]:

$$E_{\rm m} = (1 - \alpha_{mod})E_{\rm m}^{\circ} + \alpha_{mod}E_{m}^{\circ} + \gamma\alpha_{mod}(1 - \alpha_{mod})(E_{m}^{\circ} - E_{m}^{\circ})$$

$$\alpha_{mod} = \frac{\alpha - \alpha_{gel}^{mod}}{\alpha_{diff}^{mod} - \alpha_{gel}^{mod}}$$
(3)

The parameters E_m° and E_m^{∞} are the moduli of the fully uncured and fully cured resin, respectively. α_{gel}^{mod} and α_{diff}^{mod} are the extreme values of the degree of cure considered during the process and are assumed to be $\alpha_{gel}^{mod} = 0$ and $\alpha_{diff}^{mod} = 1$. The parameter γ allows quantification of the contrasting mechanisms of chemical hardening and stress relaxation. It is assumed null in this study. The instantaneous shear modulus of the resin is calculated by the relation of isotropic materials. During the process, the resin has a chemical shrinkage that induces a uniform strain for all principal directions. The mechanical properties of the fiber do not depend on the curing process and are assumed constant. The micromechanics model [6] evaluates homogeneous mechanical properties, chemical shrinkage, and thermal expansion coefficient from fiber and matrix properties.

Results

The considered laminate is 2.54 cm thick and is made of AS4/3501-6 material (graphite/epoxy). The thermophysical characteristics of the material are: $\rho = 1.52 \times 10^3 \text{ kg/m}^3$, $c_p = 942 \text{ J/}$ (W °C), k = 0.4457 W/(m °C), $A_1 = 3.502 \times 10^7 \text{ s}^{-1}$, $A_2 = -3.357 \times 10^7 \text{ s}^{-1}$, $A_3 = 3.267 \times 10^3 \text{ s}^{-1}$, $\Delta E_1 = 8.07 \times 10^4 \text{ J/mol}$, $\Delta E_2 = 7.78 \times 10^4 \text{ J/mol}$, $\Delta E_1 = 5.66 \times 10^4 \text{ J/mol}$, $H_r = 198.9 \text{ kJ/kg}$ [6]. The one-dimensional model consists of ten elements. Convection boundary conditions are applied to the top and bottom of the laminate. The first study allows the present thermochemical model to be verified by comparing the trends in the degree of polymerization and temperature at the centerline of the laminate with those predicted by Bogetti [7] for a cure cycle. The curing process consists of two hold-on periods at temperatures of 389.25 K and 450.55 K for

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70 min and 127 min, respectively. As can be seen in Fig.1(a), there is a good match between the two models. The small initial discrepancy in the degree of cure may be due to a different choice of the initial degree of cure not being specified in the reference. The temperature spikes when the air temperature is kept constant are due to the exothermic nature of the resin reaction.



Figure 1: (a) Comparison of the prediction of degree of cure and temperature for a cure cycle with Bogetti's prediction at the centreline of the laminate, (b) Degree of cure and temperature for three different cure cycles

After evaluating the model's accuracy, three cure cycles are applied to the same laminate as in the previous case. The first cycle reaches the maximum temperature of $T_1 = 453.15$ K, the second one the temperature $T_2 = 403.15$ K, and the third $T_3 = 383.15$ K and they are kept constant for 200 min. Fig. 1(b) shows the time trends of temperature and cure degree at the center of the laminate for the three cure cycles. The resin characteristics vary with the degree of cure, except for the Poisson and thermal expansion coefficients, which are assumed constant. The instantaneous resin modulus is calculated using Eq. (3) for each time step, knowing that $E_m^{\circ} = 3.447$ MPa and $E_m^{\infty} = 3.447 \times 10^3$ MPa. The fiber properties are kept constant. Through the micromechanical model, the homogeneous properties of the composite are obtained. These parameters are used as input to the analysis to calculate the deformation of an L-shaped component with an angle of 93° between the two flanges. Since the structure is symmetrical, only half is considered. The length of the single flange is 0.1 m. Refined one-dimensional kinematic model [4] can predict the structure's sping-in angle for the three cure cycles along the curvilinear coordinate x that follows the curvature of the flange. The greatest deviation of spring-in angle is obtained in the curved part of the Lshaped structure. For the three cycles the maximum values of spring-in angle are shown in Table 1.

Table 1: Maximum spring-in angle for the three cycles

| | Cycle 1 | Cycle 2 | Cycle 3 |
|-----------------------|---------|---------|---------|
| Spring-in angle [deg] | 1.02 | 0.965 | 0.939 |

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Summary

A simple one-dimensional thermochemical model made it possible to accurately predict the trends in the degree of cure and temperature of the composite given a cure cycle. If the maximum temperature of the cure cycle is low, the resin is not fully cured at the end of the process. Through the micromechanical model, it was possible to obtain the homogeneous properties of the composite as the degree of cure changes and thus obtain the inputs to derive the deformations induced by the cure cycle. A refined one-dimensional kinematic model allowed the spring-in angle to be estimated. It was shown that the cure cycle influences the spring-in angle. The deformation decreases as the maximum temperature of the cycle decreases.

Further developments may include process optimization, the development of defect mitigation methodologies, or in the development of active process monitoring strategies.

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References

[1] M. Hojjati, SV. Hoa. Some Observations in Curing of Thick Thermosetting Laminated Composites. Science and Engineering of Composite Materials, vol. 4, no. 2, 1995, pp. 89-108. https://doi.org/10.1515/SECM.1995.4.2.89

[2] G. Fernlund, C. Mobuchon, N. Zobeiry. 2.3 autoclave processing. Comprehensive Composite Materials II, Elsevier; 2018, pp. 42–62 [chapter 2]. https://doi.org/10.1016/B978-0-12-803581-8.09899-4

[3] E. Carrera, M. Cinefra, M. Petrolo, E. Zappino. Finite element analysis of structures through unified formulation. John Wiley & Sons; 2014. https://doi.org/10.1002/9781118536643

[4] E. Zappino, N. Zobeiry, M. Petrolo, R. Vaziri, E. Carrera, A. Poursartip. Analysis of processinduced deformations and residual stresses in curved composite parts considering transverse shear stress and thickness stretching. Composite Structures, Volume 241, 2020. https://doi.org/10.1016/j.compstruct.2020.112057

[5] A. C. Loos, G. S. Springer. Curing of Graphite/epoxy Composites. Technical Report AFWAL-TR-83-4040, Air Force Wright Aeronautical Laboratories, Wright Patterson AFB, OH, 1983.

[6] T.A. Bogetti, J.W. Gillespie Jr. Process-Induced Stress and Deformation in Thick-Section Thermoset Composite Laminates. Journal of Composite Materials 26. (5), 1992. https://doi.org/10.1177/002199839202600502

[7] A. Johnston. An integrated model of the development of process-induced deformation in autoclave processing of composite structures. PhD thesis. University of British Columbia, 1997.