NUMERICAL AND SEMI-ANALYTICAL MODELLING OF THE PROCESS INDUCED DISTORTIONS IN PULTRUSION

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ABSTRACT

The geometrical changes of the processed material (process induced distortions) are a critical issue in pultrusion, since they affect the process dynamics (mainly the pull force), as well as the mechanical properties and geometrical precision of the final product. Hence, a detailed understanding of the mechanical behavior generating the distortions during the process is eventually required. In the present study, two different modelling approaches are implemented and compared to calculate the development of the distortions during the pultrusion of a graphite/epoxy composite rod. In both cases, the temperature and the degree of cure distributions are obtained from the thermo-chemical analysis, using a finite element and a finite volume approach, respectively. Process induced distortions have been computed solving a sequential stress-strain finite element model, in the former case. In the latter, the transient distortions are inferred adopting a semi-analytical procedure, i.e. post processing numerical results by means of analytical methods. The predictions of the process induced distortion development using the aforementioned methods are found to be qualitatively close to each other. Furthermore, the location of the detachment between the heating die and the part due to shrinkage is also investigated.

1. INTRODUCTION

Pultrusion is a continuous manufacturing process used to realize constant cross sectional composite profiles. In recent years, the pultrusion process experienced a remarkable growing within the composite industry, due to its cost-effectiveness, automation and quality of products. Nowadays the process is widely used to manufacture highly strengthened structures such as wind turbine blades, window profiles, door panels, and reinforcement beams for concrete. In a pultrusion process, the fibers/mats are first impregnated by the (thermoset or thermoplastic) matrix material by means of a resin bath or employing a resin injection chamber. The wet out reinforcements then enter the forming and curing die where the heat activates the exothermic
reaction process. The cured profile is continuously advanced via a pulling system to the cut-off saw and finally is cut to the desired length. A schematic view of the pultrusion process is depicted in Fig. 1.

![Diagram of pultrusion process](image)

**Fig. 1. Schematic view of the pultrusion domain for the composite rod.**

Process induced shape distortions may be important for pultruded products such as window frames and fencing panels due to their desired high geometrical precision. Hence, one of the challenges in a pultrusion process is avoiding or reducing the development of process induced distortions. The transient distortions during process arise due to several mechanisms [Svanberg and Holmberg (2001), Wisnom, Gigliotti, Ersoy, Campbell and Potter (2006), Bogetti and Gillespie Jr (1992), Johnston (1997)]: (i) the mismatch in the coefficient of thermal expansion (CTE) of the matrix material and the fibers, (ii) the chemical shrinkage of the matrix material, (iii) the tool-part interaction and (iv) the temperature and the degree of cure gradients through the composite thickness due to non-uniform curing. Several numerical models have been presented in the literature, in order to achieve a better understanding of the pultrusion process [Baran, Tutum, and Hattel (2012a), Baran, Tutum, and Hattel (2012b), Baran, Tutum, and Hattel (2012c), Baran, Tutum, and Hattel (2013a), Baran, Tutum, and Hattel (2013b), Baran, Tutum, Nielsen and Hattel (2013), Carlone, Palazzo and Pasquino (2006), Carlone and Palazzo (2007), Carlone and Palazzo (2008), Joshi and Lam (2001), Joshi, Lam and Win Tun (2003), Liu, Crouch, and Lam (2000), Tutum, Baran and Hattel (2013), Valliappan, Roux, Vaughan, and Arafat (1996)].

In the present paper, two different approaches to the computational simulation of the pultrusion process have been proposed, compared and discussed. The aim of both models is to predict thermo-chemical aspects as well as process induced transient distortions in a conventional pultrusion process of a graphite/epoxy rod. The first model (Model-1) is based on the sequential coupling of a 3D Eulerian thermo-chemical model together with a 2D quasi-static plane strain mechanical analysis. The resin elastic modulus development is calculated by means of the cure hardening instantaneous linear elastic (CHILE) approach [Johnston (1997)], which is a valid pseudo-viscoelastic approximation of the linear viscoelasticity. A finite element scheme has been used to solve both boundary value problems. The second model (Model-2) is based on a semi-analytical procedure: a computational fluid dynamics (CFD) finite volume approach is employed to derive the 3D distribution of temperature and degree of cure into the processing material, while the process induced distortion are inferred post-processing numerical results by means of analytical methods. The paper is structured as follows: in Section 2 the theoretical formulation and the adopted solution strategies for the thermo-chemical boundary value problem are exposed, while in Section 3 the implemented procedure for distortion computing are detailed. Numerical outcomes are reported, compared and discussed in Section 4, briefly highlighting the most relevant conclusions in Section 5.
2. THERMO-CHEMICAL MODEL

Even if pultrusion is conceptually a very simple process, its dynamics are affected by several important aspects, such as heat and mass transfer, resin reaction and phase changes, voids growth or dissolution, interaction between the processing material and the heating die and stress-strain development. All the aforementioned issues are strictly related to thermo-chemical phenomena, which, from a modelling point of view, can be formulated in terms of energy and species balances. In more detail, the temperature distribution into the processing material can be inferred solving the following form of the energy equations:

\[ \rho C_p \left( \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x_3} \right) = k_{x_1} \frac{\partial^2 T}{\partial x_1^2} + k_{x_2} \frac{\partial^2 T}{\partial x_2^2} + k_{x_3} \frac{\partial^2 T}{\partial x_3^2} + q \]  

(1)

where \( T \) is the temperature, \( t \) is the time, \( u \) is the pulling speed (along the \( x_3 \) direction), \( \rho \) is the density, \( C_p \) is the specific heat and \( k_{x_1}, k_{x_2} \) and \( k_{x_3} \) are the thermal conductivities along \( x_1, x_2 \) and \( x_3 \) directions, respectively. Lumped material properties are used and assumed to be constant throughout the process.

The generative term \( q \) at the second member of Eq. 1 is related to the internal heat generation due to the exothermic resin reaction or conversion, i.e. the crosslinking of polymeric chains, quantified by means of the degree of cure \( \alpha \). Rigorously speaking, \( \alpha \) is defined as the ratio between the reacted species and the total reactive species at the beginning of the process, however, for convenience, it is commonly quantified considering some reaction dependent parameter, such as the released heat. Following this assumption, the degree of cure can be written as the ratio between the amount of heat \( \Delta H \), evolved up to the time \( t \), to the total heat of reaction \( \Delta H_r \) (for \( \alpha = 1 \)). As a consequence, considering that the reinforcing fibers do not contribute to the generative term and indicating the reaction rate (first derivative of the degree of cure with respect to time) as \( R_r \) it follows:

\[ q = (1 - V_f) \rho_r H_r R_r, \]  

(2)

where \( V_f \) is the fiber volume fraction and \( \rho_r \) is the resin density.

Several kinetics models have been proposed and discussed in the inherent literature to describe the evolution of the cure reaction. In the present investigation the well-established n-order model has been adopted [Valliappan et al. (1996)], assuming an Arrhenius type dependence on the absolute temperature:

\[ R_r(\alpha, T) = \frac{\partial \alpha}{\partial t} = \frac{1}{H_{tr}} \frac{dH(t)}{dt} = K_0 \exp \left( - \frac{E}{R T} \right) (1 - \alpha)^n. \]  

(3)

The above equations have been solved using a finite element scheme in Model-1. The evaluation of degree of cure and reaction rate has been obtained by means of iterative in-house developed routines implemented into the commercial software ABAQUS (version 6.11, 2011), until the matching of a temperature and degree of cure tolerance. In Model-2 a finite volume approach has been employed, defining the degree of cure as an additional volumetric scalar variable, whose transport equation, in the aforementioned hypothesis, can be written as:

\[ \frac{\partial \alpha}{\partial t} + u \frac{\partial \alpha}{\partial x_3} = R_r. \]  

(4)

Eqs. (1-4) have been solved by means of the commercial package ANSYS-CFX for Model-2.
3. CALCULATION OF THE DISTORTIONS

Model-1. The evolutions of the process induced displacements in transverse directions are predicted using a 2D plane-strain model [Baran et al. (2013)]. In this model, the cross section of the part is assumed to move along the pulling direction of the process while tracking the corresponding temperature and degree of cure profiles calculated in the 3D thermo-chemical simulation. In other words, a 3D Eulerian thermo-chemical model is coupled with a 2D plane strain Lagrangian mechanical model. The corresponding transient distortions are calculated based on the temperature and the cure distributions together with the corresponding glass transition temperature \( T_g \) of the cross section by using the quadratic plane-strain elements in ABAQUS. The instantaneous resin elastic modulus \( E_r \) development during the process is calculated using the CHILE approach [Johnston (1997)], as follows:

\[
E_r = \begin{cases} 
E_r^0 & T^* < T_{C1} \\
E_r^0 + \frac{T^* - T_{C1}}{T_{C2} - T_{C1}} (E_r^\infty - E_r^0) & T_{C1} \leq T^* \leq T_{C2} \\
E_r^\infty & T^* > T_{C2}
\end{cases}
\]  

(5)

where \( E_r^0 \) and \( E_r^\infty \) are the uncured and fully cured resin moduli, respectively. \( T_{C1} \) and \( T_{C2} \) are the critical temperatures at the onset and completion of the glass transition, respectively. \( T^* \) represents the difference between the instantaneous resin glass transition temperature \( T_g \) and the resin temperature, i.e. \( T^* = T_g - T \) [Johnston (1997)]. The evolution of the \( T^* \) is given by:

\[
T^* = T_g - T = (T_g^0 + \alpha_{T_g} \cdot \alpha).
\]  

(6)

The effective mechanical properties of the composite are calculated by using the self-consisting field micromechanics (SCFM) approach which is a well-known technique in the literature [Bogetti and Gillespie Jr (1992)]. User-subroutines in ABAQUS are used for the calculation of the transient distortions as used in [Baran et al. (2013)].

Model-2. The basic assumption of this model is that the section of the processing material varies along the pultrusion die, preserving the position of its axis of gravity (barycenter), following the approach proposed in [Joshi and Lam (2001)]. The virtual dimension (radial in this case) of \( i \)-th control volume can be computed multiplying its initial value times the correction factor:

\[
\delta_{c,i} = V_r \delta_{r,i} + V_f \delta_{f,i},
\]  

(7)

being \( \delta_{c,i} \) and \( \delta_{f,i} \) the variation of a unit dimension of the \( i \)-th volume entirely filled respectively with resin or fiber materials:

\[
\delta_{r,i} = \left(1 + \varepsilon_r (T_i - T_0)\right) \cdot \left(1 - \frac{\gamma_r \alpha_i}{100}\right)^{1/3},
\]  

(8)

\[
\delta_{f,i} = \left(1 + \varepsilon_f (T_i - T_0)\right).
\]  

(9)

In the above equation \( \varepsilon_r \) represents the thermal expansion coefficient and \( \gamma_r \) is the percentage volumetric shrinkage of the fully cured (\( \alpha = 1 \)) resin. Repeating the calculation one finally has:

\[
\Delta r_i = r_i (\delta_{c,i} - 1).
\]  

(10)

The total displacement \( \Delta_i \) can be evaluated extending Eq. 10 to the whole radius. In particular, if the virtual section of the processing composite results greater than the internal die section, i.e.
the pultruded is compressed into the die, perfect thermal contact is assumed. When the shrinkage effect prevails, inducing the detachment of the material from the die, an additional thermal contact resistance (TCR) is induced between the die and the composite. An iterative procedure connecting the thermochemical model with the dimensional change model has been used, until a temperature criterion is satisfied.

4. RESULTS AND DISCUSSIONS

The 3D thermo-chemical simulation of the pultrusion of a UD graphite/epoxy composite rod is carried out. Only a quarter of the pultrusion domain, seen in Fig. 2, is modelled due to symmetry. Instead of using the die and the heaters in the numerical model, the measured die wall temperature [Valliappan et al. (1996)] is applied to the outer surface of the rod for the length between 0-915 mm (i.e. inside the die). At the symmetry surfaces adiabatic boundaries are defined in which no heat flow is allowed across the boundaries. At the post die region, the exterior surface of the pultruded rod is exposed to ambient temperature (27 °C) assuming a temperature dependent convective heat transfer coefficient. The length of the post die region (Lpost-die in Fig. 2) is determined to be approximately 1370 mm [Valliappan et al. (1996)]. Material properties and the resin kinetic parameters are listed in Table 1 and Table 2, respectively. The parameters used in the CHILE approach for Model-1 are given in Table 3. The pulling speed is set to 5 mm/s. The inlet temperature of the composite part is assumed to be the resin bath temperature of 38 °C [Valliappan et al. (1996)] and the matrix material at the die inlet is assumed to be uncured (α = 0). In the present study, the total volumetric shrinkage of the epoxy resin is assumed to be 4% [Joshi and Lam (2001)].

![Fig. 2. Schematic view of the pultrusion domain for the composite rod. All dimensions are in mm.](image)

| Table 1. Material physical properties and concentration |
|---------------------------------|-------------------|----------------|-----------------|-----------------|----------------|
| Material                       | ρ [kg m⁻³]        | c_p [J kg⁻¹ K⁻¹] | kₜₖ [W m⁻¹ K⁻¹] | kₜₖ,ₐ [W m⁻¹ K⁻¹] | eᵦ [°C⁻¹]       | Vol. fraction |
|-------------------------------|-------------------|----------------|----------------|-----------------|----------------|
| Resin                         | 1260              | 1255           | 0.2            | 0.2             | 4.5E-5          | 0.378         |
| Fiber                         | 1790              | 712            | 66             | 11.6            | 7.2E-6          | 0.622         |

| Table 2. Resin kinetics and rheological parameters |
|---------------------------------------------------|----------------|----------------|
| K_b [s⁻¹]                                        | E [J mol⁻¹]    | H_cr [J kg⁻¹] |
| 19.14 E+4                                         | 60.5 E+3       | 323.7 E+3     |
Table 3. Parameters used in the CHILE model (Eq. 5) [Baran et al. (2013)].

<table>
<thead>
<tr>
<th>$E_r^0$ [MPa]</th>
<th>$E_r^\infty$ [MPa]</th>
<th>$T_{C1}$ [$^\circ$C]</th>
<th>$T_{C2}$ [$^\circ$C]</th>
<th>$T_g^0$ [$^\circ$C]</th>
<th>$\alpha_{tg}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>3.447</td>
<td>3.447E+3</td>
<td>165</td>
<td>215</td>
<td>0</td>
<td>380</td>
</tr>
</tbody>
</table>

The calculated centreline temperature and degree of cure profiles are shown in Fig. 3. It is seen that the predicted results match quite well with the available experimental data in [Valliappan et al. (1996)]. This shows that the present numerical schemes in Model-1 and Model-2 are stable and converged to a reliable solution. The temperature of the composite part becomes higher than the die wall temperature after approximately 380 mm from the die inlet due to the internal heat generation of the epoxy resin. At that point the peak increase rate of degree of cure is obtained. The maximum composite temperature is calculated approximately as 205 $^\circ$C. At the post die region, the degree of cure is increased slightly which indicates that the curing still takes place after the die exit. This fact was also observed in [Valliappan et al. (1996)]. The centerline degree of cure is increased from 0.838 (at the die exit) to 0.867 (at the end of the process) which corresponds to a percentage increase of approximately 3.3%.

![Fig. 3. The centerline temperature (left) and degree of cure (right) distributions.](image)

The transient distortions are calculated using the obtained temperature and degree of cure distributions in Model-1 (2D plane strain FE model) and Model-2 (1D semi analytical model). The results are depicted in Fig. 4 for the displacement evolution of the outer surface of the composite rod, i.e. the top point in Fig. 4. It is seen that the mechanical assumptions in the semi-analytical model (Model-2) with access to the calculated temperature and degree of cure developments are sufficient to obtain a trend for the transient distortions similar to the ones calculated by the finite element method (FEM) (Model-1) for the circular composite part. However, there is a significant deviation between the calculated displacements especially at the post die region in Model-1 and Model-2. As aforementioned, the SCFM approach is used in Model-1 which calculates the effective composite mechanical properties. This approach captures the mechanical response of the composite quite well [Bogetti and Gillespie Jr (1992)] such that the fibers dominate the longitudinal properties, on the other hand the transverse properties is controlled by the matrix material. For instance, the longitudinal and the transverse moduli at the end of the process are found to be approximately 130 GPa and 10 GPa, respectively in Model-1, which agrees well with typical values given in [Zenkert and Battley (2009)] for a UD carbon/epoxy with a fiber volume fraction of 60%. For the virtual displacement calculation in the transverse direction in Model-2, homogenization of the fibers and the epoxy resin variations...
is considered (Eq. 7) in terms of fiber volume fraction. Hence, the transient displacement levels are calculated relatively smaller in Model-2 if compared to Model-1. The stiffness of the epoxy resin is changed after vitrification according to the CHILE approach (see Eq. 5), hence this may cause a larger deviation in the displacement evolution at the post-die region as compared to the inside of the heating die. Inside the heating die, the simplified 1D model (Model-2) is able to predict the transient distortions with reasonable accuracy. The virtual detachment point at the die-part interface, which can be defined as the “zero” displacement during the process, is seen from Fig. 4. The detachment is found to be approximately 540 mm in Model-1 and 580 mm in Model-2 which is a good agreement between the two models. The residual displacement of the top point in Fig. 4 is calculated approximately as -0.025 mm and -0.017 mm for Model-1 and Model-2, respectively.

Fig. 4. The process induced transient displacements in the x_2-direction.

5. CONCLUSIONS

In the present work, the transient distortions were predicted using a 2D plane strain FE model (Model-1) and a 1D semi-analytical model (Model-2). The temperature and the degree of cure distributions are first calculated at steady state and good agreement was found between the two models. Using these temperature and degree of cure profiles, the transverse displacement evolution of the composite surface was predicted. A similar trend of development was obtained using the two models since the process induced variations were defined based on the thermal expansion and chemical shrinkage. The displacement levels in Model-2 were found to be close to the ones obtained in Model-1 inside the heating die. For the post die region, the deviation between the two results has become larger since the effect of the matrix material on the distortion behavior in the transverse direction is more pronounced in Model-1 as compared to Model-2.

ACKNOWLEDGEMENTS

This work is a part of DeepWind project which has been granted by the European Commission (EC) under FP7 program platform Future Emerging Technology.
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