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CRediT authorship contribution statement

Michael Sandberg: Conceptualization, Methodology, Software, Validation, Formal analysis, Visualization, Writing - Original Draft, Onur Yuksel: Investigation, Writing - Review & Editing, Ismet Baran: Investigation, Writing - Review & Editing, Jon Spangenberg: Investigation, Supervision, Writing - Review & Editing, Jesper H. Hattel: Investigation, Methodology, Project administration, Funding acquisition, Writing - Review & Editing
Steady-state modelling and analysis of process-induced stress and deformation in thermoset pultrusion processes

Michael Sandberg\textsuperscript{a,}\textsuperscript{*}, Onur Yuksel\textsuperscript{b}, Ismet Baran\textsuperscript{b}, Jon Spangenberg\textsuperscript{a}, Jesper H. Hattel\textsuperscript{a},

\textsuperscript{a}Department of Mechanical Engineering, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark
\textsuperscript{b}University of Twente, Faculty of Engineering Technology, NL-7500AE Enschede, The Netherlands

Abstract

Process-induced stress and deformation are critical factors when ensuring product quality and structural integrity of composite profiles manufactured using thermoset pultrusion processes. In this paper, we present a new steady-state 3D-Eulerian numerical framework that enables 9-35 times faster computations compared to the current state-of-the-art quasi-static 3D-methods. In addition, we show how process-induced effects from the profile-advancing pulling force and an initial compressive stress state can be modelled. We demonstrate in theoretical parameter studies that the pulling force advances die-detachment and reduces die-swelling, while the initial compressive stress state has the opposite but a more pronounced effect.

Keywords: Pultrusion; thermo-chemical-mechanical modelling; composite processing; residual stresses; process-induced deformation; streamline integration; Eulerian solid mechanics

1. Introduction

Pultrusion is an efficient, cost-effective, and high-output manufacturing technology to mass-produce fibre-reinforced polymer (FRP) composite profiles with a constant cross section [1–4]. Pultruded profiles benefit from having a high and consistent product quality and the processing steps generate almost no waste, since there is no required use of consumables such as vacuum bags, flow media, etc. While pultrusion only represented 4.7% of the European FRP composite market in 2017 (0.055 of 1.118 million tonnes), it was the fastest-growing sector wrt. production output (+6%) [5]. A descriptive illustration of the pultrusion process is given in Fig. 1 (in Sec.
In thermoset pultrusion processes, a low-cost and fast-cure resin system is critical to achieving a high production output at a reasonable cost. These much-desired properties are enabled by a strong exothermic cure reaction and a powerful heating configuration, which in turn comes with the cost of chemical cure shrinkage and thermal gradients in the composite part. If these effects are not controlled, the composite part may not achieve the desired product quality due to process-induced defects such as curing-cracks or shape distortions (warpage). Therefore, engineers seek to analyse the effect of process-induced stress and deformation in early design stages by use of simulation models.

### 1.1. Literature

#### 1.1.1. Thermo-chemical-mechanical (TCM) modelling of composite manufacturing processes

The process-induced strains that give rise to stress and deformation during processing are associated with the thermal and cure history that the composite part experiences during the processing steps. While the consti-
tutive mechanical behaviour of the fibre reinforcement is considered to remain constant within normal process
conditions, phase changes of a thermoset resin system must be described with an appropriate constitutive model.

The "cure-hardening instantaneously linear elastic" (CHILE) approach introduced by White and Hahn [6]
and Bogetti and Gillespie [7] is a simplified approach to describe the constitutive mechanical behaviour of a
fibre-reinforced polymer composite during processing. The CHILE model is an incremental linear elastic model
in which the elastic modulus of the resin system changes instantaneously with curing. CHILE models can be
enriched with a temperature-dependent term that describes thermal-softening of the resin system [8]. CHILE
models are sometimes referred to as pseudo-viscoelastic models, as the instantaneous modulus reflects the time
span or frequency it was measured at. Compared to true viscoelastic models, CHILE models are incapable
of predicting time-dependent constitutive mechanical behaviour of composite parts during processing [9–11].
Nonetheless, the numerical framework in this paper is based on the CHILE approach as it remains popular in
the composite industry and research [12–19] (pultrusion processes included) due to its reasonable simplicity in
implementation and material characterisation. We refer to Baran et al. [11] for an extensive review of TCM
modelling of composite manufacturing processes.

1.1.2. TCM modelling of pultrusion processes

Heat-transfer analysis, which is the starting point for a TCM model, has been conducted numerically and ex-
perimentally of pultrusion processes by several researchers in literature. Examples can be found for the conven-
tional resin-bath pultrusion processes (RBP) [20–25], resin-injection pultrusion processes [26–30], pultrusion
of thermoplastic pre-impregnated materials [31, 32], and out-of-die UV-cured pultrusion processes [33–35].

TCM modelling of pultrusion processes was first introduced by Baran et al. in 2013. The idea behind Baran
et al. [15]’s original work was to use the thermal and cure history that a 2D-cross section of the profiles sees
during the process as input to the subsequent mechanical analysis (Table 1(a)). This approach allows one to
perform a segregated quasi-static transient mechanical analysis by using a conventional TCM framework in the
Lagrangian frame (the cross-section that follows a material point of the profile) [7, 8], while the thermo-chemical
analysis is carried out in an Eulerian frame (the full profile, as in conventional thermo-chemical methods [20–
23]). The original work in Baran et al. [15] relied on 2D plane strain assumptions, but it has later been extended
Baran et al. [15]’s original work has been the basis for several theoretical and experimental investigations on how process-induced stress and deformation in pultrusion processes are affected by the process conditions for a number of different profiles, resin systems, and fibre layups. Besides a square bar that served as a case study in [15, 16], researchers have studied process-induced stress and deformation of pultruded L-shaped and rectangular hollow profiles (Baran et al. [17, 36]), aerodynamic NACA airfoil profiles for vertical axis wind turbine blades (Baran et al. [18]), and thick composite rods (Safonov et al. [37]). In the referred work, [17, 36, 37], the authors reported process-induced deformations and cracks observed from industrially pultruded profiles, and recently, residual stresses in pultruded profiles have been investigated by use of digital-image-correlation and hole-drilling experiments by Yuksel et al. [38, 39].

Table 1: Methodologies behind the current state-of-the-art 2D-3D and 3D-3D TCM models (a-b) that couple the Eulerian and Lagrangian methods. Figs. (a-b) illustrate how the coupling between the Eulerian and Lagrangian frames works by letting a cross section or part of the profile (Lagrangian frame) travel through the temperature- and cure-history (Eulerian frame) with velocity, $v_{pull}$. Fig. (c) illustrate the main principle behind this paper in which displacements rates are determined in the Eulerian frame and accumulated along streamlines of the material flow. Figs. (a-c) depicts one-quarter of the stationary temperature field in a thermoset pultrusion process, where the symmetry about the $x_1$, $x_2$- and $x_1$, $x_3$-planes has been exploited.

1.1.3. Steady-state mechanical modelling

Baran et al. [15]’s original work laid the groundwork for TCM simulation of pultrusion. This initial approach, however, relied on interpolation between two separate domains and it was limited to a reduction of the actual 3D displacement field. While Baran et al. expanded the original method to 3D in [16], we will demonstrate in this paper that the needed intermediate time stepping in a quasi-static analysis results in an inefficient approach for iterating towards a stationary solution in 3D.
To overcome the drawbacks mentioned above, one has to determine the process-induced stress and deformation in the same Eulerian frame as the temperature and cure degree fields. While Eulerian approaches are typically seen as reserved for fluid mechanics rather than solid mechanics, other researchers have already benefited from utilising similar methods to model process-induced stress and strain in a variety of continuous manufacturing processes. These examples include friction stir welding (Bastier et al. [40], Arora et al. [41]), plate rolling (Nielsen et al. [42]), wire drawing (Juul et al. [43]), etc. Modelling pultrusion, being a continuous manufacturing process, can also benefit from using a similar approach. Instead of iterating towards a stationary solution through time-stepping in a Lagrangian quasi-static analysis (Baran et al. [15, 16]), process-induced stress and deformation can be calculated everywhere at once by utilising a stationary Eulerian approach. As we will demonstrate in this paper, a fully Eulerian approach allows for 3D analysis of process-induced stress and deformation in pultrusion processes at a fraction of the computational cost of the established Eulerian-Lagrangian methods.

1.2. Scope and overview

The scope of this paper is to present a new numerical framework that is based on a steady-state Eulerian formulation to model process-induced stress and deformation in pultrusion processes. In the paper, we further expand the framework to consider: i) surface tractions introduced by contact towards the pultrusion die that contribute to the pulling force; and ii) an initial compressive stress state perpendicular to the pulling direction from, e.g. the bulk compaction of the fibre material needed to achieve the desired volume fraction or a resin pressure state induced during resin impregnation.

The paper is structured as follows. Section 2 starts by describing the proposed numerical framework that is outlined in Table 2. The numerical framework is validated using data from the literature in Section 3. Finally, Section 4 summarises the conclusions of the paper.

2. Method

The case study in this paper was based on the original experimental work by Chachad et al. [44] that also served as the basis for Baran et al. [15, 16]. The case study concerned pultrusion of a square orthotropic
Table 2: Architecture and the main steps in the algorithm of the numerical framework. The contour plots in the table exemplify stationary solutions in a thermoset pultrusion process where the symmetry about the $x_1$, $x_2$- and $x_1$, $x_3$-planes has been exploited. The contour plot of $T$ depicts both the profile and pultrusion die, while only the profile is depicted for the remaining variables. The theoretical background for the solution steps is described in Sec. 2. Sec. 2.5 summarises the solution steps.

<table>
<thead>
<tr>
<th>Step</th>
<th>Variables solved for (selected examples)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Step 1: Thermo-chemical analysis: Calculate heat-transfer and resin cure (Solve for variables $T$, $\alpha$ cf. Sec. 2.2)</td>
<td></td>
</tr>
<tr>
<td>Step 2: Incremental mechanical analysis: Calculate displacement rates (Solve for variable $\dot{u}_i$, Sec. 2.2.1). See Sec. 2.3.2 for implementation of mechanical contact towards the die walls and Sec. 2.4 for further possible extensions.</td>
<td></td>
</tr>
<tr>
<td>Step 3: Post-processing: Perform integration along streamlines to accumulate any desired output variable, e.g. all components of process-induced deformation ($u_i$), strain ($\varepsilon_{ij}$), and stress components ($\sigma_{ij}$) along streamlines (Sec. 2.3).</td>
<td></td>
</tr>
</tbody>
</table>

Figure 1: (Not to scale) Cut-view of the case study. The figure illustrates how the impregnated fibre material enters from the left of the pultrusion die, where the resin cure is controlled by active heating and cooling. The die is $L_D = 0.915$ m long with a wall thickness of 25.4 mm. While heating or cooling is not applied to the first 60 mm of the pultrusion die, three evenly spaced 270 mm long heater units cover the top of the die. A 135 mm long cooler is placed below the first heater unit. The square profile is 25.4 mm thick and drawn from left to right. As the figure illustrates, die-detachment and die-swelling can simultaneously take place at different locations of the profile.

2.1. Material derivative and streamlines

When using a conventional Lagrangian formulation, which is the basis of the state-of-the-art mechanical models in Baran et al. [15, 16], incremental changes such as process-induced deformation, strain, and stress...
rates are associated with a material point of the profile. In an Eulerian formulation, which is the basis of the new approach in this paper, incremental changes are associated with the spatial variation along a streamline. These rates are described by use of the material derivative (Eq. (1)) that relates the rate of change of a physical quantity moving along a streamline with velocity \( v_i \):

\[
\dot{()} = \frac{\partial()}{\partial t} + v_i \frac{\partial()}{\partial x_i} = (),_t + v_i (),_i
\]  

(1)

Note that throughout the paper, repeated indices imply summation and we employ both (),_i and \( \partial() / \partial x_i \) to denote partial differentiation. Since we seek stationary solutions, temporal terms, \( \partial() / \partial t = () ,_t = 0 \), are omitted.

When a model of a pultrusion process is restricted to a number of conditions that reflect conventional pultrusion processes, the velocity components and the associated streamlines that compose the material derivative are readily available. This is the case when all streamlines follow the \( x_1 \)-axis (as indicated in Fig. 2), and only the profile-advancing pulling speed contribute to the velocity \( v_1 = v_{\text{pull}} \) given that:

- the pultrusion die is straight. Alternatively, any process-induced stress and deformation that may take place in a non-straight part of the die are negligible (e.g. through a section where the die tapers);
- in resin-injection pultrusion processes, any process-induced stress and deformation that takes place near inlet ports are negligible due to the low cure state of the resin;
- any process-induced deformation can be described by small strain theory (Cauchy’s strain/stress) and equations are solved in the undeformed configuration.

### 2.2. Thermo-chemical model

Stationary equilibrium in the Eulerian frame for the conservation of energy and species (degree of cure) implies:

\[
\frac{\partial}{\partial x_i} (K_{ij} \frac{\partial T}{\partial x_j}) + v_{\text{pull}} \rho c_p \frac{\partial T}{\partial x_1} = S_T, \quad v_{\text{pull}} \frac{\partial \alpha}{\partial x_1} = R_\alpha
\]  

(2)

where \( T \) is the temperature and \( \alpha \) is the degree of cure. \( K_{ij} \) and \( \rho c_p \) are effective thermal conductivity tensor and thermal capacities, respectively. The cure-rate, \( R_\alpha \), is temperature- and cure-dependent, and the heat generated
in the exothermic reaction, $S_T$, is proportional to the cure-rate. These relationships, together with relevant material data, are summarised in Table 3 (Appendix A). The convective term (e.g. the 2nd term in Eq. 2) entered when applying the material derivative (Eq. 1) to the temporal term ($\dot{T} = v_{pull} \partial T / \partial x_1$, etc.).

2.2.1. Process-induced strain rates

The process-induced strain rate was considered as an additive decomposition of the thermal expansion and chemical cure shrinkage that the resin system exhibits during cross-linking: $\dot{\varepsilon}^{pr}_{ij} = \dot{\varepsilon}^{ch}_{ij} + \dot{\varepsilon}^{th}_{ij}$. The rate of process-induced thermal expansion is related to the rate of temperature change, and the effective thermal expansion coefficients ($\alpha^{th}_{ij}$, Table 3) of the composite part:

$$\dot{\varepsilon}^{th}_{ij} = \alpha^{th}_{ij}\dot{T} = \alpha^{th}_{ij}v_{pull} \frac{\partial T}{\partial x_1} \quad (3)$$

In Eq. (3), the material derivative (Eq. (1)) was inserted to obtain the spatial gradient of the temperature ($\dot{T} = v_{pull} \partial T / \partial x_1$). The process-induced strain rate introduced by chemical shrinkage is related to the cure rate:

$$\dot{\varepsilon}^{ch}_{ij} = \alpha^{ch}_{ij}\varepsilon^{ch}_{r} \quad (4)$$

where the material derivative was utilised to obtain the spatial gradient of the degree of cure and $V_{sh}$ is the volumetric shrinkage of the resin after complete cure. The coefficients, $\alpha^{ch}_{ij}$, relating the isotropic resin shrinkage and the anisotropic shrinkage, are listed in Table 3.

2.3. Mechanical model

The stress rates, $\dot{\sigma}_{ij}$, are related to the strain and displacement rates through a conventional constitutive relation:

$$\dot{\sigma}_{ij} = L_{ijkl}(\dot{\varepsilon}_{kl} - \dot{\varepsilon}^{pr}_{kl}), \quad \dot{\varepsilon}_{ij} = \frac{1}{2}(\dot{u}_{i,j} + \dot{u}_{j,i}) \quad (5)$$

where the elastic part of the strain rate tensor was found via an additive decomposition of the total strain rate and the process-induced strain rates $\dot{\varepsilon}^{e}_{kl} = \dot{\varepsilon}_{kl} - \dot{\varepsilon}^{pr}_{kl}$. The entries of the instantaneous stiffness tensor, $L_{ijkl}$, were based on the self-consistent field micromechanics (SCFM) for an orthotropic layup by Bogetti and Gillespie [7]. The instantaneous resin modulus was described with an enhanced CHILE model that included thermal softening.
Finally, the evolution of glass temperature, $T_g$, was described with a Di Benedetto equation [45]. These relationships are summarised in Table 3.

Force equilibrium was based on stress rates rather than total stress since the numerical framework was based on the incremental constitutive CHILE model:

$$\dot{\sigma}_{ij,j} = 0$$  \hspace{1cm} (6)

In Eq. (6), body forces and mass inertia were omitted. It is important to note that the operations needed to establish and solve Eq. (6) are not in any way different from the equilibrium equation of total stresses that is solved in commercial FEM programs.

2.3.1. Streamline integration

Rate-measures must be accumulated along streamlines to obtain the total measures of process-induced stress, strain, or deformation. This operation can be resembled by the integral (cf. Table 1(c)), which, for example, yields for the thermal-induced strains:

$$\epsilon_{ij}^{th} = \frac{1}{v_{\text{pull}}} \int_{x_{1,1}}^{x_{1}} \epsilon_{ij}^{th} \, dx$$  \hspace{1cm} (7)

The solution to this integral was obtained by solving a convective-type equation where the strain rate entered as source term similar to the energy and species equations (Eq. (2)):

$$v_{\text{pull}} \frac{\partial \epsilon_{ij}^{th}}{\partial x_1} = \epsilon_{ij}^{th}$$  \hspace{1cm} (8)

2.3.2. Mechanical contact towards the die walls

If the process-induced chemical shrinkage exceeds the thermal expansion, the profile may detach from the die walls. This condition poses an inequality constraint that must be treated with an appropriate mechanical contact formulation. Even though most commercial software packages come with options to address this elementary contact condition, built-in functions may prove unsuitable or incompatible due to the intermediate step of streamline integration (Sec. 2.3.1) needed to obtain the total displacements from Eqs. (5-6). When this is the case, we suggest enforcing the contact condition using a simple variation of the active-set strategy (see e.g.
Wriggers and Zavarise [46]) which is detailed in Appendix B and used throughout the paper. Please note that when not otherwise stated, the contact condition was considered adhesion- and friction-free corresponding to the assumptions in Baran et al. [15, 16].

### 2.4. Possible extensions

Although a simulation framework that is based on the solution steps listed in Table 2 and detailed in Secs. 2-2.3.2 is capable of simulating all the features of the original work by Baran et al. [15, 16], the following three subsections describe possible extensions that reflect additional physics that take place in pultrusion processes. These extensions also exemplify some of the additional modelling possibilities when the mechanical response is not limited to a 2D reduction of the displacement field. It is important to note that these extensions are theoretical modifications of the original framework. Therefore, until the proper experimental evidence is present, results produced using the extensions detailed in Secs. 2.4.1-2.4.3 represent hypothesised process behaviour.

#### 2.4.1. Release of free stresses upon die-exit

For a boundary with a surface normal, $n_i$, stress equilibrium in solid mechanics implies that $\sigma_{ij}n_jn_i = 0$ when no surface tractions are applied (no force/flux leaves or enter a free and undisturbed surface, see e.g. Fig. 1 in Heller et al. [47]). In conventional solid mechanics problems solved with finite elements methods, this constraint automatically enters as a so-called natural or non-essential boundary condition (see e.g. Cook et al. [48]). However, since this work was based on the equilibrium of stress rates (Eq. 6), it was needed to enforce this constraint as a boundary condition to the stress rates. Therefore, when the profile pushes towards the die walls, this boundary condition "releases" the corresponding stress state upon exiting the die. We found that adding a Neumann-type boundary condition (flux) on free surfaces that penalises normal stress as a manageable way to implement this constraint$^1$:

$$\sigma_{ij}n_i n_j = a_{pen}\sigma_{ij}n_i n_j \quad \text{(on free surfaces of the profile outside the die)}$$  \hspace{1cm} (9)

As with any penalty approach, the penalty factor, $a_{pen}$, must be set to an appropriate level that correctly

$^1$In Sandberg et al. [30], Appendix C, we derive how a penalty term enters as a Neumann-type boundary condition.
enforces the desired boundary condition. A too-small penalty factor may not sufficiently enforce the desired
constraint, and a too-large factor may result in state matrices becoming ill-conditioned or the solution unstable.
A parameter study (Fig. 2) revealed that a penalty factor between 2 and 20 was the optimal choice for the
process conditions in the case study. Throughout the remainder of this paper, $\alpha_{pen}$ was set to 10. As Fig. 2
indicates, the result of this boundary condition is that the profile may swell and expand upon exiting the die.
This post-die response reflects the well-known phenomenon "die-swell" or "extrudate-swell" that is commonly
observed in polymer extrusion processes with and without fibre-reinforcement (e.g. Heller et al. [47], Ganvir
et al. [49]). Please note that the die-swell is the result of releasing compressive stress ($\sigma_{ij}n_in_j < 0$) upon
die-exit. Releasing a tensile stress state would result in rapid contraction upon die-exit, but this cannot take
place when the contact towards the die walls is considered adhesion-free (cf. Sec. 2.3.2).

![Figure 2: Example of how the constraint violation for $\sigma_{33}$ (at the top of the profile) after the exit of the die is affected by the penalty factor, $\alpha_{pen}$. The Snippets (a-d) depict the vertical displacement, $u_3$ inside and outside the die (marked dark grey and white, respectively) as free stresses are released. As it can be seen in the figure, a penalty factor that is too small does not fully release the free stresses (a-b), while a too high penalty factor introduces oscillations in the solution near the die-exit (d).](image)

2.4.2. Pulling-force induced tractions from profile to die wall contact

As the raw material is drawn through the die, bulk compaction, viscous drag, and mechanical sliding friction
towards the die walls build up a resistance force that must be overcome to advance the profile. This force is
the "pulling force" ($F_p$ in Fig. 1) that is applied to the profile to control the output rate (pulling speed) of the
production. While the magnitude of the pulling force depends on the profile dimensions, material system, and
process conditions, the capacity of industrial pulling mechanisms is reported to range from 3 to 24 tonnes (or
approximately 30 to 240 kN) [1]. An applied load of this magnitude contributes to the process-induced strain
and stress state in the profile, and this is relevant to examine. Although it is outside the scope of this paper to define the various contributions to the pulling force (see e.g. [1, 3, 50–52]), we discuss how to include pulling-induced surface traction parallel to the pulling direction in the equilibrium equation for the stress rates (Eq. 6).

The traction induced by contact to the pultrusion die ($f_\parallel$ in Fig. 1) must be enforced as a rate-measure:

$$\dot{\sigma}_{ij} s_i n_j = v_{pull} \frac{\partial f_\parallel}{\partial x_1} \quad \text{(on the outer surface of the profile inside the die)}$$

(10)

where $s_i = (1, 0, 0)$ is a vector along the pulling direction and parallel to the outer surfaces of the profile. The rate-measure of $f_\parallel$ was obtained by utilising the material derivative in Eq. (1). For velocity-dependent traction, $f_\parallel$, proportional to the pulling speed (e.g., the case with viscous drag), $v_{pull}$ would be squared on the right-hand side of Eq. (10) after applying the material derivative.

Please note that outside the pultrusion die, there is no surface traction, $f_\parallel = 0$. Since this condition, together with the chemorheological behaviour of the resin system, can introduce a discontinuity in $f_\parallel$, we found that it was necessary to approximate the spatial derivative in Eq. (10) by using the shape functions of the finite element framework.

2.4.3. Inclusion of an initial compressive stress state perpendicular to the pulling direction

In pultrusion processes, the resin system normally saturates the fibre reinforcement at an overpressure. The overpressure is achieved by tapering a section of the pultrusion die, or by resin injection at elevated pressure. The resin pressure typically ranges between 5 to 30 bar (0.5 to 3 MPa) [1]. In addition to the resin pressure, bulk compaction of the fibre material introduces a stress state when it enters the pultrusion die. For reference, based on the through-thickness compaction tests by Sandberg et al. [53], a compaction pressure of approximately 7.5 bar (0.75 MPa) is needed to achieve the volume fraction of the test case ($V_f = 0.639$, cf. Table 3).

It must be noted that the initial stress states of the resin system and fibre material are, of course, affected by the subsequent processing steps. For example, the resin pressure decreases as it flows through the fibre material, and stress-relaxation will take place during solidification. Similarly, the fibre material exhibits time-dependent stress-relaxation, also when the resin system lubricates it. For simplification, we will only use a sequential
approach where a fraction of the resin pressure and fibre stress is assumed to enter as an initial condition to
the subsequent stress analysis upon entering the pultrusion die. Please note that this is a simplification since
an integrated flow-stress model is needed to calculate the effective load transfer from the impregnation flow
and fibre compaction. It is outside the scope of the paper to integrate these capabilities into this new numerical
framework, so we refer to Niaki et al. [54, 55, 56] for more information about the topic.

To apply the stress state at the entrance of the pultrusion die, it entered as a boundary condition in the
streamline integration scheme (Eqs. (7-8)). Thereby, to obtain the total accumulated stress components, $\sigma_{22}$ and
$\sigma_{33}$, one must set (exemplified for $\sigma_{22}$):

$$v_{\text{pull}} \frac{\partial \sigma_{22}}{\partial x_1} = \dot{\sigma}_{22} \quad (\sigma_{22} = \sigma_\perp \text{ at } x = x_{st}) \quad (11)$$

As Eq. 11 indicates, only a stress state perpendicular to the pulling direction, $\sigma_\perp$, will be considered, since it
is reasonable to neglect the pressure contribution in the $x_1$-direction because of the high axial stiffness of the
profile. It is noted that $\sigma_\perp$ must not violate stress equilibrium (i.e. the equivalent of Eq. (6)) when enforced
using this approach.

2.5. Solution strategy

The governing equations were solved with the continuous Galerkin finite element method in the commer-
cial simulation software package, COMSOL Multiphysics® [57]. We employed second-order elements for the
solution of displacements and displacements rates (for Eq. (6), serendipity elements were used), and for the
remaining equations, first-order elements were used. Convective terms were stabilised using COMSOL’s built-
in streamline and crosswind diffusion schemes. Throughout the model, numerical integration with $2 \times 2 \times 2$
gauss-points was utilised. The mesh-discretisation is depicted in Fig. 3.

The model utilised three segregated solution steps in accordance with Table 2. Step 1 consisted of calculating
the stationary temperature and degree of cure fields ($T$ and $\alpha$, respectively, in Eq. (2)). From $T$ and $\alpha$, the resin
modulus, the associated stiffness tensor ($E_r$ and $L_{ijkl}$, respectively, in Appendix B), and the process-induced
strain rates ($\dot{\epsilon}_\text{ch}^{ij}$ and $\dot{\epsilon}_\text{th}^{ij}$ in Eqs. (3-4)) were determined and used as input in Step 2 to calculate the displacements
rates ($\dot{u}_i$ in Eq. (6)). In the case that die-detachment was considered, Step 2 included an intermediate step where
the total transversal displacements, \( u_2 \) and \( u_3 \), were used as input in the iterative contact formulation (Sec. 2.3.2 and Appendix B). If the release of free stresses after the die-exit was considered, the transversal stress components, \( \sigma_{22} \) and \( \sigma_{33} \), needed to be calculated together with the displacement rates, \( \dot{u}_i \), to enforce stress-release upon die-exit (Sec. 2.4.1). In post-processing, Step 3, desired rate-variables were accumulated along streamlines to interpret results (Sec. 2.3).

![Figure 3: The mesh-discretisation near the pultrusion die. The snippets illustrate the through-thickness element distribution and mesh refinement near the exit of the die. The simulation model included approximately one metre before and nine metres after the pultrusion die that is not shown in the figure.](image)

3. Results

3.1. Stationary fields and validation of the numerical framework

Stationary solutions of temperature, degree of cure, as well as process-induced strain, stress, and deformation are depicted in Figs. 4 and 6a. Results from Baran et al. [15, 16] are highlighted with a black-dotted line to validate the numerical framework. While these figures confirmed that the numerical framework was able to reach the same results from [15, 16], we discuss the different responses in the following paragraphs to provide context for the remainder of the paper.

As the profile entered the pultrusion die, the top of the profile quickly approached the set-temperature of the heater units (Fig. 4). Approximately three-fourths into the die, the temperature at the centre of the profile exceeded the top. This temperature increase was caused by the low thermal conductivity of the profile itself as well as the strong exothermic heat reaction of the resin system. Upon exiting the die, the profile was cooled by convective heat transfer to the ambient surroundings. At distances 0.69 and 0.87 metres after the die-exit (top
Following the rise in temperature and degree of cure, process-induced strains started to accumulate. In the $x_1$-direction (the fibre and pulling direction), almost no contraction due to chemical shrinkage was obtained ($\epsilon_{11}^{ch}$ in Fig. 4). This response was expected since only the resin system contributes to the chemical shrinkage, and the structural response of the composite profile in the $x_1$-direction was dominated by the high stiffness of the fibre material. Compared to the $x_1$-direction, the process-induced strains in the $x_2$ and $x_3$-directions (transversal to the fibre direction) were approximately ten times higher.

Due to the through-thickness temperature gradient in the profile, the elevated temperature at the top introduced a local compressive $\sigma_{11}$-component. As a result, to achieve net stress equilibrium in the $x_1$-direction, a tensile $\sigma_{11}$-component developed in the centre of the profile. While this relationship between tensile and compressive stresses switched for approximately two meters after the die-exit as the profile solidified, it remained towards the end of the process.

The die-walls constrained expansion of the profile in the $x_2$ and $x_3$-directions. Since the thermal expansion exceeded the chemical shrinkage inside the die, this confinement resulted in compressive stress components, $\sigma_{22}$ and $\sigma_{33}$ (-0.2 MPa or approximately 2 bar), at the centre and top of the profile. Towards the exit of the die, a tensile $\sigma_{22}$ component was observed at the top of the profile.

Finally, in accordance with Baran et al. [15], approximately 28 mm before the die-exit, the corner of the profile detached from the die walls (see Snippet (II) in Fig. 6a).

3.2. Computation times

The elapsed time for the computation of the case study in Sec. 3.1 and the other examples throughout the paper lasted less than five minutes for a mesh containing 20000 elements (6-core i7-8300K @3.7 GHz with 64 GB ram). To benchmark the performance of the new numerical framework against the Eulerian-Lagrangian approaches in Baran et al. [15, 16], the computations were repeated with mesh resolutions from 8,000 to 33,000. See Fig. 5. Please note that the Eulerian-Lagrangian frameworks from Baran et al. [15, 16] were rebuilt in COMSOL Multiphysics and we ran all computations on the same computer to obtain a fair comparison of the computational efficiency.
Figure 4: Temperature, degree of cure, stress, and strain probed at the centre (blue) and the top (red) of the profile. In Baran et al. [16, Figs. 10 and 11], the authors reported different results for their plane strain and generalised plane strain 2D reductions, as well as their full 3D Eulerian-3D Lagrangian model. While the temperature, degree-of-cure, and process-induced strains are unaffected by any 2D reduction imposed on the displacement field, the lengthwise stresses, $\sigma_{11}$, are not; in this figure, all results are compared to the full 3D Eulerian-3D Lagrangian model from [16] (shown as the dotted line “Ref.”), since these results do not rely on a 2D reduction of the displacement field. Please note that the single ref. point presented for $\sigma_{11}$ “top” was taken from Baran et al. [16, Fig. 15].
As Fig. 5 illustrates, the new numerical framework was $9 - 35 \times$ faster than the 3D Eulerian-3D Lagrangian method based on Baran et al. [16]. While no direct comparison can be drawn to the 3D Eulerian-2D Lagrangian method (Baran et al. [15]) since its mechanical response was based on a 2D-reduction of the displacement field, it is worth mentioning that computations were actually $1.5 - 3 \times$ faster than the new numerical framework presented in this paper. Thus, it is evident that the 3D Eulerian-2D Lagrangian method remains as an attractive approach due to its computational efficiency.

The new Eulerian numerical framework achieves this attractive computational efficiency since a steady-state analysis needs no intermediate time-steps. While the quasi-static Eulerian-Lagrangian approaches took approximately 100 intermediate steps to reach the stationary solution, the new numerical framework only needed three to four iterations related to enforcing the contact condition towards the die walls (Appendix B). We do, however, acknowledge that intermediate time steps are in fact of interest when investigating transient solutions during start-up or time-dependent process conditions. As such, there is not the same basis for achieving a similar speed-up by utilising an Eulerian formulation in transient analyses.

![Graph](image.png)

Figure 5: Elapsed computation times on a workstation PC (6-core i7-8300K @3.7 GHz with 64 GB ram) for several mesh resolutions (8,000 to 33,000 elements). In the figure, 3D Eulerian-2D Lagrangian refers to computations using the original method by Baran et al. [15] and 3D Eulerian-3D Lagrangian is using the 3D extension in Baran et al. [16]. The exponents to $N_e$ indicate the slope of the exponential fits. The multiples in the figure are approximate.

3.3. Extensions

3.3.1. Release of free stresses after die-exit

Fig. 4 shows that a compressive $\sigma_{33}$-component towards the die walls remained throughout the pultrusion die (see also Baran et al. [15, Fig. 10(c)]). This behaviour indicated that the profile pushed against the die walls,
and as a result, we observed a rapid expansion at the top and sides of the profile after the die-exit (see Snippet (I) in Fig. 6a and the deformed cross-sectional shapes in Fig. 6b). The expansion also materialised in a positive bulk response upon die-exit (Fig. 6b). In polymer extrusion processes with and without fibre-reinforcement, this post-die response is commonly referred to as "die-swelling" or "extrudate swell"\(^2\), but it has, to the authors’ knowledge, not yet been reported for pultrusion processes. While this post-die response only took place when the stress release was considered, we were able to reach the same conclusions when adaptive time-stepping and a nonlinear Newton-Raphson solver were used in our implementation of the original quasi-static 3D Eulerian-2D Lagrangian framework by Baran et al. [15] (see the dash-dotted line in Snippet (I), Fig. 6).

\[ \text{Figure 6: (a) Process-induced deformation probed at the top and corner of the profile. The dash-dotted line in Snippet (I) depicts the obtained displacement in the } x_3 \text{-direction we obtained from the 3D Eulerian-2D Lagrangian method with a total stress formulation from Baran et al. [15]. Snippet (II) reveals the detachment point, which matched the reported value in [15] (0.88 m). (b) Cross-sectional averaged volumetric strain } \Delta V/V = \epsilon_{ii} \text{. The snippet of the cross-sectional averaged longitudinal and transverse strain components show that only the } \epsilon_{11} \text{-component contributed to the cross-sectional averaged volumetric strain inside the die. Fig. (b) also shows the cross-sectional deformation at five selected locations (magnified } \times 50) \text{ with and without the release of free stresses.} \]

3.3.2. Effects of process-induced tractions from die wall contact

In this example, a pulling force between approximately 0 and 10 tonnes \( (F_p = 0 \ldots 100 \text{ kN}) \) was assumed to materialise in an evenly distributed traction, \( f_{\parallel} \), over the contact area towards the die walls. As discussed in Sec. 2.4.2, this range reflects the reported capacity of low to medium-sized industrial pulling mechanisms, according to Starr [1].

\(^2\)For example, Fig. 1 in Heller et al. [47] illustrates that the die-swelling is associated with enforcing the normal stress component towards the free surface, \( \sigma_{ij}n_in_j = 0 \)
As a natural consequence of the pulling force, the $\sigma_{11}$-component started to build up as the profile advanced through the pultrusion die (Fig. 7a). The magnitude of $\sigma_{11}$ reflected the applied pulling force distributed over the cross-sectional area of the profile. Likewise, the shear stress near the die walls corresponded to the evenly distributed traction, $f_{\parallel}$ (Snippet (I) in Fig. 7a). The pulling force also induced axial extension of the profile. This extension resulted in transversal contraction due to the effective Poison’s ratio of the profile. As a consequence, we observed that the detachment from the die walls in the corner was advanced approximately 20 mm when the pulling force was increased (Snippet (I) in Fig. 7b). Moreover, the die-swelling at the top of the profile was reduced by approximately 2 $\mu$m (Snippet (II) in Fig. 7b). While the magnitudes of these reported effects were limited, they would be more pronounced for a profile with a lower degree of mechanical anisotropy (wrt. the effective Poison’s ratios for the 1, 2 and 1, 3-directions).

3.3.3. Effects of an initial compressive stress state perpendicular to the pulling direction

In this example, the profile response includes a small fraction of the resin pressure and bulk fibre compaction as an initial stress state perpendicular to the pulling direction, $\sigma_{\perp}$. Based on the discussed magnitudes in Sec. 2.4.3, a parameter study of $\sigma_{\perp} = 0 \ldots 0.2$ MPa was conducted.

The $\sigma_{22}$ and $\sigma_{33}$-components increased inside the pultrusion die in accordance with the initial stress state.
perpendicular to the pulling direction (see the snippet (I) in Fig. 8a). Consequently, the detachment point from
the die walls was delayed (snippet Fig. 8b) and the die-swelling at the top increased ($\approx 0.1$ mm, Fig. 8b for $\sigma_\perp = 0.2$ MPa). In fact, die-swelling at the corner of the profile was observed for all the different initial stress
states considered, and the profile always remained pushed against the die walls throughout the process.

Since the resin modules first developed at the sides and corners of the profile (see $E_r$ in the snippet in Fig. 4),
the increased initial stress state was carried by the circumference of the profile after the die-exit. Consequently,
we observed limited effects on the deformation at the corner of the profile ($u_2$ in Fig. 8b), but a significant
increase wrt. to the transversal stress component at the top of the profile ($\sigma_{22}$ in Fig. 8a). In the centre of the
profile, the resin modulus was low upon die-exit. This softness of the profile core permitted lateral displacement
of the sides of the profile, which meant that the stress state had a pronounced effect on the observed die-swelling
($u_3$ in Fig. 8b).

Figure 8: Effects on an initial stress state perpendicular to the pulling direction, $\sigma_\perp$: (a) Transversal stress components, $\sigma_{22}$ and $\sigma_{33}$; (b) Vertical displacement at the top, $u_3$, and horizontal displacement at the corner, $u_2$, of the profile.

### 3.4. Closing remarks

The CHILE model in the case study (Table 3) included three stages (two constant moduli with one inter-
mediate linear phase). Other studies that have utilised CHILE models in pultrusion processes have included
an additional intermediate stage to characterise an exponential rise in stiffness during the liquid and gel phases
[36, 58]. However, since CHILE is an incremental linear elastic model, it cannot capture the true viscoelastic
behaviour of the resin system during its liquid and gel phases. This limitation extends to the SCFM micromechanics model by Bogetti and Gillespie [7], which only reflects the effective elastic behaviour of the composite.

The assumptions and simplifications of the CHILE and SCFM models may lead to results that are not always reflected by the expected physical behaviour of the profile during the processing steps. For example, the constitutive behaviour of the resin system in its liquid and gel phases is characterised by a high bulk modulus, but the shear modulus is low (see Péron et al. [59] for an example of an Epoxy resin system). Essentially, at a low degree of cure, the resin system will flow when subject to loading. The compressive strength of the composite is also highly dependent on the shear strength of the polymer (Budiansky and Fleck [60]), making the composite prone to fibre buckling.

The aforementioned points are essential to note since stress built up before the resin system reached the glass-transitioning temperature. In particular, the stress build-up in the $x_1$-direction at low degree-of-cure (governed by the through-thickness temperature gradient and shearing), must but overestimated (Figs. 4 and 7(a)). In addition, the reported die-detachment and die-swelling took place before reaching the glass-transitioning temperature. Therefore, these phenomena are also subject to the simplifications of the constitutive model. Further research utilising viscoelastic constitutive models that are proven accurate above the glass-transitioning temperature are needed to study these phenomena in depth.

4. Conclusions

In this paper, we presented a new steady-state 3D-Eulerian numerical framework for the analysis of process-induced stress and deformation in thermoset pultrusion processes. We highlight the following conclusions of using the numerical framework and findings of the parameter studies in the paper:

- Compared to the existing 3D state-of-the-art methods, we showed that computations using our new approach was between $9-35 \times$ faster in the examples presented;
- While the existing literature has reported the possibility of having the profile detaching from the die, we found that compressive stress towards the die-exit can result in die-swelling, which is a commonly reported phenomenon in e.g. polymer extrusion processes;
A parameter study revealed that the pulling force advanced the detachment point from the die walls and decreased die-swelling. On the other hand, an initial stress state associated with bulk fibre compaction or impregnation flow had a more pronounced but oppositve effect.

Since the die-detachment and die-swell took place before the glass-transition temperature was reached in the case study, a topic for future research could be to apply constitutive models that are more suitable for capturing viscoelastic effects in the liquid and gel phases of the resin system.

### Appendix A - Material models and parameters

<table>
<thead>
<tr>
<th>Physics, component or feature</th>
<th>$K_{11}$ [W/(m K)]</th>
<th>$K_{22,33}$ [W/(m K)]</th>
<th>$c_p$ [J/(kg K)]</th>
<th>$\rho$ [kg/m$^3$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Composite (lumped for $V_f = 0.639$)</td>
<td>0.9053</td>
<td>1.04</td>
<td>797.27</td>
<td>2090.7</td>
</tr>
<tr>
<td>Die</td>
<td>40</td>
<td>40</td>
<td>460</td>
<td>7833</td>
</tr>
</tbody>
</table>

Cure kinetics (Eq. (2))

$$R_\alpha = A_0 \exp \left( \frac{-E_a}{RT} \right) (1 - \alpha)^n f(\alpha, T) [1/s]$$

with temperature- and cure-dependent diffusion factor: $f(\alpha, T) = 1/(1 + \exp[30(\alpha - (1.5 + 0.0055T)]) [-]$

<table>
<thead>
<tr>
<th>Heat reaction (source term in Eq. (2))</th>
<th>$\rho_c$ [kg/m$^3$]</th>
<th>$H_c$ [kJ/kg]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_T = (1 - V_f) \rho_c H_c$</td>
<td>1260</td>
<td>275 · 10$^3$</td>
</tr>
</tbody>
</table>

Resin modulus

$$E_r = \begin{cases} E_r^0 & T < T_G & 4.47, 3.447 \\ E_r^\infty & T > T_G 
\end{cases}$$

Resin temperature (Di Benedetto equation)

$$T_{G\infty} - T_{G0} = \frac{\alpha_{T}}{1 - (1 - \alpha)\lambda}$$

Constitutive relations

$$E [MPa] \quad \nu [-] \quad G [MPa] \quad \alpha [1/K]$$

Glass (fibre reinforcement, ) $f$, isotropic

$$73.08 \cdot 10^3 \quad 0.22 \quad 29.92 \cdot 10^3 \quad 5.04 \cdot 10^{-6}$$

Epox (resin, $r$, isotropic)

$$0.35 \quad E_r/(2(1 + \nu_r)) \quad 5.76 \cdot 10^{-5}$$

Composite ($V_f = 0.639$)$^1$

<table>
<thead>
<tr>
<th>$\varepsilon_{11}$</th>
<th>$\varepsilon_{22}$</th>
<th>$\varepsilon_{33}$</th>
<th>$\varepsilon_{12}$</th>
<th>$\varepsilon_{13}$</th>
<th>$\varepsilon_{23}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1/E_{11}$ $\nu_{12}/E_{11}$ $\nu_{13}/E_{11}$</td>
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<td>0</td>
<td>0</td>
<td>$\varepsilon_{11}$</td>
<td></td>
</tr>
<tr>
<td>$1/E_{22}$ $\nu_{23}/E_{22}$</td>
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<td>0</td>
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<td>$\varepsilon_{33}$</td>
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<td>$\nu_{23}$</td>
<td>$\nu_{33}$</td>
<td>$\nu_{12}$</td>
<td>$\nu_{13}$</td>
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</table>

<table>
<thead>
<tr>
<th>$\sigma_{11}$</th>
<th>$\sigma_{22}$</th>
<th>$\sigma_{33}$</th>
<th>$\sigma_{12}$</th>
<th>$\sigma_{13}$</th>
<th>$\sigma_{23}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$1/(G_{12})$</td>
<td>0</td>
<td>0</td>
<td>$\varepsilon_{11}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$1/(G_{13})$</td>
<td>1</td>
<td>0</td>
<td>$\varepsilon_{22}$</td>
<td></td>
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</tr>
<tr>
<td>$1/(G_{23})$</td>
<td>0</td>
<td>1</td>
<td>$\varepsilon_{33}$</td>
<td></td>
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</tr>
</tbody>
</table>

Effective expansion/contraction coef. of composite$^2$

$$\alpha_{ij}^\mathrm{eff} = \frac{\alpha_{ij}}{E_{ij}(1-V_f)} \quad (1 - \nu_r)(1 - V_f) - (\nu_r V_f + \nu_r(1 - V_f))\alpha_{11}^\mathrm{th}$$

Chemical contraction coef., $\alpha_{ij}^\mathrm{ch}$

$$\frac{\alpha_{ij}}{E_{ij}(1-V_f) + \alpha_{ij}E_r(1-V_f)} \quad (\alpha_f + (1 + \nu_r) V_f + \alpha_r + V_f(1 - V_f))\alpha_{11}^\mathrm{th}$$

Thermal expansion coef., $\alpha_{ij}^\mathrm{th}$

$^1$For brevity, the constitutive relation is given as the compliance tensor instead of the stiffness tensor, $L_{ijkl}$ (its inverse). The entries, $E_{11}, G_{12}, \nu_{12}, ...$, were estimated based on the self-consistent field mechanics methods (SCFM) by Bogetti and Gillespie [7] for transversely orthotropic laminates.

$^2$Off-diagonal terms are zero (thermal/chemical).
Appendix B - Active set contact formulation

The active set contact formulation is an iterative approach in which contact is defined using a local variable, \( \Gamma_c \), on contact surfaces. In this work, when \( \Gamma_c = 1 \), the displacement rate was set to zero. The variable was updated iteratively as it was checked if the profile penetrated \((u_i n_i > 0)\) or adhered \((\sigma_{ij} n_i n_j > 0)\) to the die-walls. If any of these conditions were fulfilled, the local value of the active set variable was set to zero from this point and downstream, \( \Gamma_c = 0 \). If \( \Gamma_c \) did not change throughout an iteration, convergence was assumed. Fig. 9 summarises these operations. Throughout the examples in this paper, convergence was achieved within 3-4 iterations.

Initialize active set: \( \Gamma_c^{(0)} = 1 \)

Set: \( \Gamma_c^{(n)} = \Gamma_c^{(n-1)} \)

Solve: \( \dot{u}_i, \sigma_{22}, \) and \( \sigma_{33} \).

Integrate along streamlines to obtain \( u_2 \) and \( u_3 \).

Penetration in non-active set \((u_i n_i > 0)\)?

No

Remove from active set by setting \( \Gamma_c^{(n)} = 0 \) when \( \sigma_{ij} n_i n_j > 0 \) in \( \Gamma_c^{(n)} = 1 \)

End step

Yes

Add to active set by setting \( \Gamma_c^{(n)} = 1 \) when \( u_i n_i > 0 \) in \( \Gamma_c^{(n)} = 0 \)

Negative reac. in active set \((\sigma_{ij} n_i n_j > 0)\)?

No

Yes

Figure 9: Flow chart of the active-set contact methodology to model how the profile may detach from the die wall due to chemical shrinkage
Acknowledgements

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Data availability statement

The processed data required to reproduce these findings are available in Fig. 1 and Table 3.


Declaration of interests

☒ The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

☐ The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: