NUMERICAL OPTIMIZATION AND SENSITIVITY ANALYSIS OF PULTRUSION PROCESS PARAMETERS

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Abstract

The purpose of this study is to develop methods of numerical optimization and sensitivity analysis of pultrusion process parameters. With this object in mind, a mathematical model of material behavior is implemented within ABAQUS environment, accounting for the dependence of matrix thermomechanical characteristics (elasticity moduli, CTE's, heat capacity and heat conductivity) on the temperature and the degree of polymerization. Modeling methods developed allow a researcher to predict of temperature, degree of curing and stress–strain distributions in a part during pultrusion process. For numerical optimization and sensitivity analysis of process parameters, a special simulation scheme was developed in pSeven software suite. pSeven is a platform for automation of engineering simulation and analysis tasks, multidisciplinary optimization and data mining. As an example, the process of pultrusion of GFRP (glass fiber reinforced plastic) rod with diameter of 80 mm is presented. The optimization parameters are the initial temperature of resin, temperatures in the 1-st and the 2-nd die zones, and pulling speed. To find optimum manufacturing parameters following constraints are considered: transverse stresses in the pultruded rod, maximum temperature of material, maximum temperature and degree of cure at the end (cut-off) section of the profile. As a result of optimization, guidelines on manufacturing process conditions have been developed allowing a pulling speed increase of 24 % to be achieved satisfying all constraints.

1. Introduction

Today, complex shape pultruded profiles of GFRP are widely used in aerospace, railway, construction and other industries. Examples of such components include structural elements of composite bridge structures (beams, bridge decking, girders etc.), elements of aircraft structures, elements of power line supporting structures, high voltage insulators etc.

Being rather expensive compared to structures made of traditional structural materials such as wood, concrete and metals, polymer composite structures can nevertheless successfully compete with their traditional counterparts in many applications, especially where the weight or corrosion resistance of a structure is a decisive factor. However they also have to remain cost effective. One way of achieving this goal is through optimization of manufacturing process, maximizing production rate at a given quality of components produced. The task of producing items of specified quality is usually solved experimentally (by trial-and-error method) through variation of manufacturing process parameters. Such iterative procedure can be quite expensive, labor-intensive, and ineffective, especially in case of large components, thus making the development of mathematical models allowing optimization of

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manufacturing parameters based on simulation of chemical and thermomechanical processes taking place in a component during fabrication an urgent problem.

2. Pultrusion

Pultrusion in principle is a process where a continuous reinforcement (glass fiber roving and tapes) is pulled through an impregnation bath containing thermoset resin and then fed into a heated forming die determining the geometry of pultruded profile cross section and where resin cure takes place (Fig. 1).

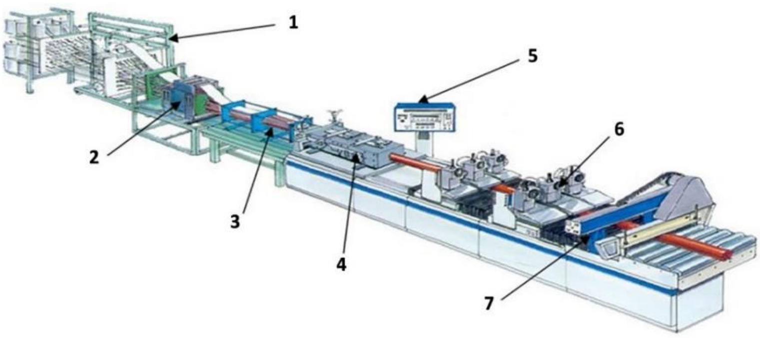

Figure 1. Pultrusion process layout: 1 – creels with reinforcement, 2 – impregnation bath, 3 – preforming (folding) unit, 4 – forming die, 5 – control panel, 6 – pulling unit, 7 – cut-off unit.

Several studies on the application of numerical and experimental methods for thermochemical analysis of pultrusion process have been conducted earlier [1-3], investigating the distribution of temperatures and cure degree profiles within the heated forming die.

The investigation of the thermo-mechanical aspects of pultrusion process, such as changes in mechanical properties, deformations and stresses developing in a profile during pultrusion, has been made by Baran et al. [4]. The approaches applied in [3] were adopted from the works investigating thermo-mechanical aspects of some non-pultrusion processes of composite structures fabrication (autoclave curing, vacuum infusion, and closed die injection), featuring common mechanism of residual stresses / strains evolution, similar to that of pultrusion process [5, 6].

3. Outline of process simulation

To adequately describe changes occurring in a preform during manufacturing process (as it passes through the heated die), following phenomena should be taken into account: the transfer of heat within a composite material; chemical reaction of polymerization; internal release of energy during chemical reaction; temperature and chemical deformations within a preform; thermal and mechanical contact with die surfaces; changes of thermal and mechanical properties of composite material, resulting from phase transformations in a resin.

Consider a steady state motion of an infinite body of a uniform cross section along x-direction with a speed V, as it undergoes a reaction of polymerization accompanied by a release of heat. All points of a body are assumed to move linearly with a constant velocity. The body is heated as it passes through the heated forming die and is cooled down after exiting the die. The ambient temperature, temperature field distribution over the die surface, temperature and degree of polymerization at the die entrance are known.

Temperature field distribution within a pultruded profile is modeled using heat transfer equation:

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$$C\rho V\frac{\partial T}{\partial x}=\lambda_x\frac{\partial^2 T}{\partial x^2}+\lambda_y\frac{\partial^2 T}{\partial y^2}+\lambda_z\frac{\partial^2 T}{\partial z^2}+q, \tag{1}$$

where x – lengthwise coordinate, y, z – cross section coordinates, V – pulling speed, T – temperature, C – heat capacity of a composite material, ρ – density of a composite material, λ – heat conductivity, q – rate of heat release during reaction of polymerization. Thermal characteristics (specific heat capacity and heat conductivity coefficients) depend on the temperature and on the attained degree of polymerization.

A distinctive feature of modeling the behavior of thermoset matrix composites is a necessity to determine phase state changes in a resin over time. To characterize phase state changes occurring in a resin a degree of cure, α, (changing in the range from 0 to 1) is used. Degree of polymerization rate of change depends on the temperature and the attained degree of polymerization and can be described by the following equation:

$$q=\rho_m H_{tot}\frac{d\alpha}{dt}\left(1-V_f\right), \tag{2}$$

where ρ_m – density of thermoset matrix; H_{tot} – specific heat (per unit mass) released at complete polymerization; $d\alpha/dt$ – rate of reaction of polymerization; V_f – volume fraction of reinforcement in a composite material.

Mechanical properties of resin change during matrix solidification. For the purpose of the present work the Poisson’s ratio of resin is assumed to remain constant (as in [4]), while the Young modulus E_m is calculated as follows:

$$E_m(T^*)=\begin{cases} E_m^0, & T^*<T_{C1} \\ E_m^0+\dfrac{T^*-T_{C1}}{T_{C2}-T_{C1}}\left(E_m^\infty-E_m^0\right), & T_{C1}\le T^*\le T_{C2}, \\ E_m^\infty, & T^*>T_{C2} \end{cases} \tag{3}$$

here $T^*=T_g-T$, where T_g – glass transition temperature depending on the degree of cure and determined from the following equation (see [6]):

$$T_g(\alpha)=T_{g0}+\left(T_{g\infty}-T_{g0}\right)\frac{\lambda\alpha}{1-(1-\lambda)\alpha}, \tag{4}$$

Here T_{g0}, $T_{g\infty}$, λ, T_{C1}, T_{C2}, E_m^0, E_m^∞ – material constants determined experimentally.

For stress determination a model of transversely isotropic material is used, where stiffness tensor depends on a phase state of resin (elastic, solid) and changes during polymerization process. Stiffness tensor at each instant of time is determined as follows: first, the Young modulus of resin is calculated using the equation (4), and then the effective characteristics of composite material are calculated based on the micromechanical model. Mechanical and thermal properties of reinforcing fibers are assumed to remain constant over time.

The model described above (1)–(4) is implemented within ABAQUS environment by means of the user subroutine mechanism. Thermal conductivity equations are solved using standard ABAQUS tools.

4. Computational model of a pultrusion of a large diameter rod

In this study the process of pultrusion of GFRP rod of 80 mm diameter is simulated. A distinguishing feature of this process is that it takes a substantial amount of time to fully heat-up a pultruded body to the temperature of polymerization reaction initiation. If process is organized such that bulk polymerization of a pultruded profile is completed within a forming die, the required pulling speed will be unreasonably low. Moreover, during polymerization the resin releases heat which is expended for

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additional heat-up of pultruded body. This can result in a large temperature surge within a central part of pultruded profile and, hence, in a local thermal destruction of material.

The situation is different when large diameter rods are fabricated with a higher pulling speed. Only outer layers of pultruded profile are able to heat up and polymerize within a forming die (Fig. 2). After the forming die exit internal layers of pultrusion continue to heat up due to a heat released during polymerization of outer layers of pultrusion. When internal layers of pultruded profile reach the temperature of polymerization a polymerization reaction starts, accompanied by a release of heat. After exiting the forming die a pultruded profile may undergo formation of mainline cracks. Formation of cracks is associated with temperature stresses forming within a polymerized part of pultruded profile (Zone 2) as a result of high temperature gradients forming after hot profile exits the forming die (see Fig. 3). Also, formation of main cracks is facilitated by high internal hydrostatic pressure of uncured resin (Zone 1), resulting from the pressure applied at the die entrance to squeeze excess resin and the additional pressure due to a temperature increase. If the thickness of already polymerized outer layers after the die exit is sufficient to withstand temperature stresses and internal hydrostatic pressure of uncured resin, formation of mainline cracks in a pultruded profile during polymerization of internal layers can be avoided. Hard solid case of polymerized external layers contacting with die surfaces prevents formation of mainline cracks. However, at a very high pulling speed a hard case of polymerized material has no time to gain thickness and strength sufficient to withstand internal hydrostatic pressure and stresses.

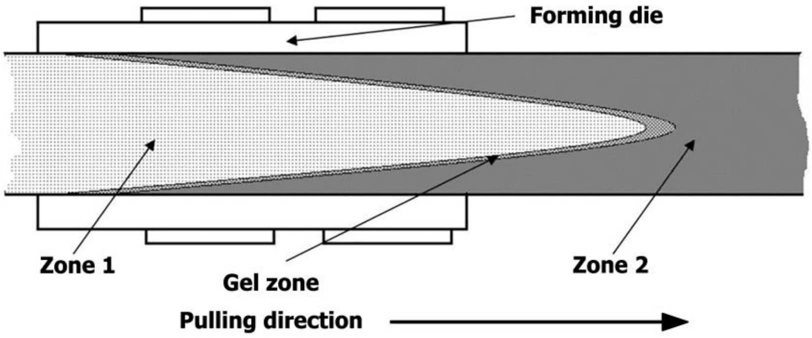

Figure 2. Polymerization in a pultruded rod during pulling.

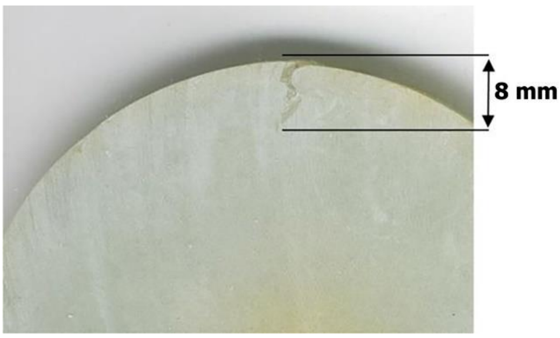

Figure 3. Cross section of a pultruded rod at a location of a crack.

It has been found experimentally that mainline cracks in pultruded profiles start to form at a distance of 10–15 cm from the die exit. After initiation a mainline crack quickly propagate over the surface of pultruded part in the direction of the die and further into the die. After a certain period of time, a leakage

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of uncured resin from a crack can be observed, indicating the presence of unpolymerized phase inside the pultruded profile after the die exit. The description of parameters used in the developed mathematical model of heat conductivity, polymerization and stress-strain state during pultrusion of a rod of 80 mm diameter is given in [7].

5. Study of computational model and optimization

The computational model can be used to study behavior of the system and to solve problems of finding optimum processing parameters. For the purpose of such studies an automated computational workflow has been created in pSeven suite developed by Datadvance company [8]. Two goals are considered within this report:

- Determination of parameter space areas satisfying or violating certain quality constraints;
- Optimization of process parameters to maximize production rate, while satisfying all relevant constraints.

Model behavior is analyzed in relation to parameters listed in Table 4.

Table 4. Process parameters and measuring ranges.

Parameter	Symbol	Lower boundary	Upper boundary
Pulling speed, mm/s	u	0.75	1.5
Initial temperature, °C	T_0	20	50
Temperature in Die zone 1, °C	T_1	140	170
Temperature in Die zone 2, °C	T_2	170	200

Computational model allows determination of a large number of physical properties of the pultruded profile. Criteria considered in this study are shown in Table 5.

Table 5. Physical restrictions

Characteristic	Restriction	Motivation
Maximum temperature of material	< 200 °C	To prevent thermal degradation
Maximum temperature at cut-off section	< 90 °C	To allow sufficient cooling of profile at cut-off
Minimum degree of polymerization at cut-off section	> 90 %	To ensure completion of polymerization by cut-off
Maximum transverse stress	< 11 MPa	To prevent cracks formation

To determine and visualize areas of constraint violations an approximation model was built in pSeven suite, allowing prediction of product characteristics for various combinations of processing parameters. The model was built using 120 data points uniformly distributed within the space of parameters given in Table 4. The algorithm based on Gaussian processes is used, allowing sufficiently accurate models to be built based on relatively small samples [9]. Accuracy of the model (RRMS, relative root mean squared) determined using points of a training sample is as follows: maximum temperature – 0.01; temperature at cut-off section – 0.02; degree of polymerization – 0.027; maximum stress – 0.075. The model allows determination and mapping of constraints violation areas within the parameter space. Such maps may be useful for manufacturing engineers choosing optimum process parameters. Figure 4 shows 2D sections of models in "pulling speed vs initial temperature" coordinates within ranges given in Table 4, for different temperatures in the 1-st and the 2-nd die zones.

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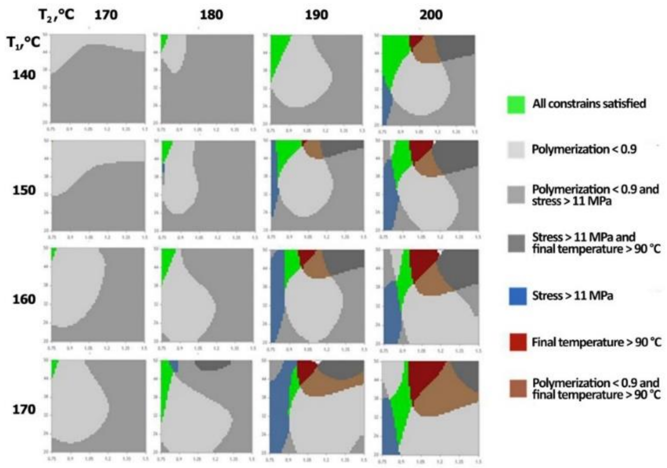

Figure 4. Areas of constraint violations

It can be seen that allowable speed values do not reach the boundaries of prescribed measuring range at any values of other parameters. Also it can be concluded that at minimum die temperatures there exists no parameter configuration satisfying all constraints. The integral sensitivity of product characteristics to changes in process parameters has been determined based on the sample used. The results are shown in Figure 5 in a shape of normalized contribution of each parameter to the variation of function.

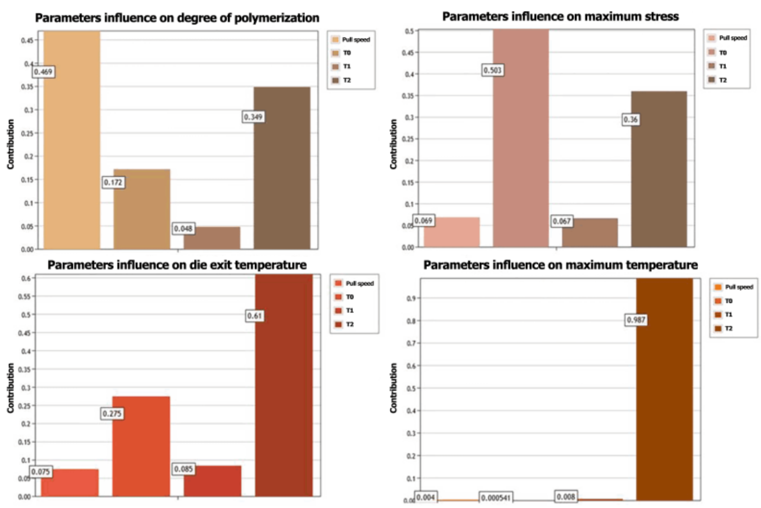

Figure 5. Sensitivity to parameter changes

Optimization problem is solved in two statements. In a single criterion statement it is required to maximize pulling speed while satisfying prescribed constraints. A two-criteria problem statement intends to maximize pulling speed and degree of polymerization simultaneously. In this case a solution will be a Pareto front of optimum configurations. A metamodels based SBO (surrogate based optimization) algorithm is used for optimization. One of the main areas of SBO algorithms application is computationally expensive problems when a solution has to be found within the frames of specified computational budget. SBO algorithms begin with large distances within the space of optimized parameters and move to small distances. At the initial stage of optimization the whole parameter space is investigated within the frames of the allocated computational budget, and meta-models are built for functions of the problem, approximating dependencies studied. By default, pSeven utilizes its own

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hierarchical models based on the theory of random gaussian processes. Built models are used to find next candidates for evaluation.

Evaluation results for established candidates are used to refine metamodels and the process is continued iteratively. A metamodel based algorithm was also used to solve two-criteria problem [10]. Figure 6 shows the optimization history where one can clearly see two stages of searching for optimum solution, related to initial investigation of parameters space and subsequent refinement of optimum location. Allocated computational budget is 100 evaluations.

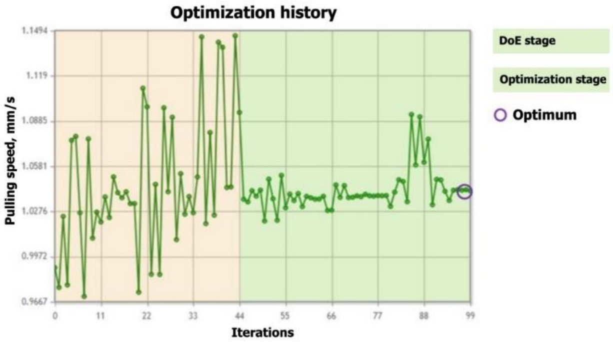

Figure 6. Optimization history.

One can clearly see that in optimum configuration the initial temperature and the temperature in the 1-st die zone have maximum allowable values. A degree of polymerization and a temperature of material at a cut-off section are used as operating constraints. As a result of optimization a pulling speed increase of 24 % has been achieved compared to initial configuration.

In a two-criteria problem a pulling speed and a degree of polymerization at the profile cut-off section are maximized simultaneously. In this statement a solution is a front of Pareto-equivalent configurations. The application of MOSBO (multi-objective surrogate-based optimization) algorithm of pSeven algorithms library allows an approximation of Pareto-front to be obtained within a small number of iterations. Allocated computational budget for this optimization problem is 100 evaluations, using data of additional 60 data points evaluated earlier. Figure 7 shows all points found during optimization and Pareto-frontier points in "pulling speed vs. degree of polymerization" coordinates, together with initial configuration.

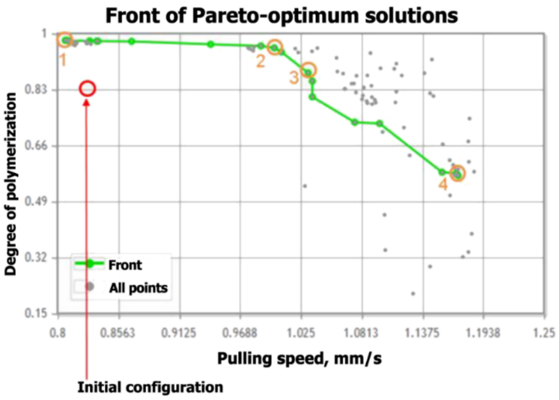

Figure 7. Pareto front.

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Obtained frontier allows a comparison of different Pareto-equivalent configurations to be made. It should be noted that Pareto front point corresponding to the degree of polymerization of 0.9 fits a solution of single criterion problem with corresponding constraints. Table 6 shows the values of parameters, objective functions and constraints for marked points of Pareto front and for initial configuration.

Table 6. Front points

	Parameters					Constraints		
	u, mm/s	α	T_0, °C	T_1, °C	T_2, °C	T_{end}, °C	T_{max}, °C	σ, MPa
Constraints	0.8–1.2		20–70	120–170	150–200	...–90	...–210	...–11
Initial	0.83	0.83	40	150	180	73	180	10.1
Point 1	0.80	0.98	64	142	197	76	196	10.6
Point 2	0.99	0.96	66	144	194	89	194	10.4
Point 3	1.03	0.89	62	160	176	89	176	9.1
Point 4	1.2	0.57	58	166	168	89	167	10.2

6. Conclusions

A computational model of pultrusion process allowing determination of physical characteristics of pultruded profile for a wide range of process parameters is presented. Allowable parameter configurations satisfying manufacturing criteria are studied based on modeling data. A problem of process parameters optimization to maximize pulling speed was solved in various statements. For the optimum configuration found a pulling speed increase of 24 % was achieved compared to initial configuration. Based on results obtained a conclusion can be made that methods of numerical simulation and optimization may be successfully used to find optimum process parameters in composite manufacturing.

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