

COMPUTER METHODS IN MATERIALS SCIENCE

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CFD (COMPUTATIONAL FLUID DYNAMIC) OPTIMIZATION STRATEGY APPLIED IN PULTRUSION PROCESS

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Abstract

Pultrusion is a composite manufacturing process in which fibers are pulled continuously through a resin bath for resin impregnation before entering in a heated die, where an exothermic cure reaction occurs. The thermal energy necessary to the reaction system depends upon many aspects such as cure kinetics and pulling speed. Generally, six rectangular heaters are coupled on the pultrusion die surface to heat the material. In the present work, it was possible to check that the energy rate can be largely reduced by changing this usual heating configuration. A new configuration based on an internal heating with smaller superficial area was simulated by a CFD model. The results were compared with experimental results from the reported literature and showed that the proposed configuration was able to cure the material in efficient way. In order to find the minimum energy rate we used a particle swarm optimization algorithm.

Key words cure reaction, polymer composites

1. INTRODUCTION

Composite materials can be used effectively for structural applications where high strength-to-weight and stiffness-to-weight ratio are required (Santos et al., 2009). Polymeric composites are manufactured by different processes, such as pultrusion, hand lay up, filament winding, etc. The pultrusion process consists in pulling continuous roving and/or mats through a resin bath and then into a heated die where the profile is cured continuously and acquires the shape of the die cavity (Voorakaranam et al., 1999). The die may be heated by electrical heaters, strip heaters, hot oil or by steam, although electrical heaters are the most common ones (Meyer, 1985). Outside the die, the composite part is pulled by a continuous pulling system and then a cut-off saw cuts the part into a desired length. Figure 1 shows a scheme of pultrusion equipment.

The degree and uniformity of cure influence composite mechanical properties. A non-uniform distribution of degree of cure in the cross section of the material implies a product of unreliable quality (Coelho et al., 2002). Variables, such as die temperature, pulling speed, pulling force, internal pressure and resin cure kinetics, control the composite process during the pultrusion. Among these variables, the die temperature (the temperature imposed on the die wall) is the most relevant one for obtaining a part with uniform and excellent mechanical properties (Coelho et al., 2002). At the beginning of the cure, it is necessary to heat the system in order to initiate the cure reaction. At this stage, the heat transfer occurs from the die wall to the center of the material. During the process, heat is generated by the cure reaction and there is a crossing point where the heat transfer direction is inverted (Basuki et al., 1998; Liu & Hillier, 1999). It is important to control the temperature using a minimum heating flux on each stage of the process. of the results corresponded to the expected behavior of the process, some aspects are incomplete in these works (Han et al., 1986; Santiago et al., 2003), regarding to the temperature profile on the die wall imposed as a boundary condition. They did not explain what the correspondent heater arrangement



Fig. 1. Scheme of pultrusion equipment (Santos et al., 2009).

In the present investigation, a numerical procedure based on CFD technique for a threedimensional simulation of pultrusion process was developed. The heater arrangement on the die wall and its influence on the energy consumption were studied here. The development of a new heating strategy to reduce the energy consumption in the pultrusion process is the main objective of this work.

2. Prior work on modeling and simulation

A number of researchers solved the non linear differential equations that represent the physical phenomena of a pultrusion process. The die-heating environment is the region considered in the modeling. Han et al. (1986) were one of the first researchers to simulate pultrusion. The finite difference method was applied to solve the equations and the temperature distribution of the composite could be obtained. The influence of the reaction inside the die cavity on the degree of cure and on the temperature profiles was explained in the simulation. The researchers affirmed that the cure kinetics needs to be known in order to configure all the other parameters: velocity, temperature and the necessary amount of catalyst added in the reaction system. Santiago et al. (2003) simulated, by finite element method, the pultrusion process of a cylindrical composite. Despite necessary to generate such temperature profile would be.

Some researchers have simulated the pultrusion by using finite element (FE) packages to perform heat-transfer and mass-transfer analyses. The FE packages are appropriate to model irregular shapes in three-dimensions and a variety of boundary conditions and material properties can be defined easily. Moschiar et al. (1996) simulated the pultrusion process by using a die with three heat zones described by three heaters along die length. Li et al. (2001) considered the simulation of three heaters on the top and three on the bottom of the die wall. Srinivasagupta et al. (2003) affirmed that the number of heating zones is variable, but three are found to be sufficient in practice. All these authors (Moschiar et al., 1996; Li et al., 2001; Srinivasagupta et al., 2003) have used this heater arrangement to model the pultrusion process of composites with different dimensions and properties. However, no attention was given to the effects of heater arrangement changes on the necessary thermal energy and composite quality.

Some researchers have optimized the pultrusion process based on a minimization of an objective function. Generally, this function represents the economy of the process. In this case, the optimum temperature profile imposed on the die surface has to be found by minimizing energy consumption. Srinivasagupta and Kardos (2004) used a thermodynamic objective function to minimize the energy consumption during the cure reaction. They and Joshi et al. (2003) considered that the number and geometry of the heaters were previously known before the numerical optimization. However, the heater geometry has strong influence upon the desired optimum results. Electrical heaters with wide superficial area may spend thermal energy excessively to cure the material. Therefore this aspect must be studied in the pultrusion optimization.

3. Numerical procedure

3.1. Balance Equations

Heat transfer in the pultrusion process can be modeled using the energy equation and a cure reaction model. In this study, it was assumed a steady state condition and a cylindrical cross section composite profile.

The three-dimensional energy balance can be expressed as:

$$\rho_c C_{p_c}(u_i \nabla T) = k_c \nabla^2 T + C_{a_0}(1 - \phi) \Delta H_t R_a \qquad (1)$$

where *T* is the temperature, u_i the pulling velocity at (*i*) direction, C_{p_c} , k_c and ρ_c are composite specific heat, thermal conductivity and density respectively, ΔH_t is the total heat generated by the cure reaction, R_a is the reaction rate of the resin, ϕ is the fiber volume fraction, C_{a_0} is the resin initial concentration.

In the pultrusion, fibers are saturated with resin before entering the heated die. It is reasonable to assume that the cure time is higher than the resin flow time. Thus, there is no need to consider the momentum equation. The mass balance, in terms of concentration, may be expressed as:

$$\frac{d\alpha}{dt} = R_a \tag{2}$$

where α is the degree of cure. In this case, *z* is the distance from the die entrance measured along the die axis as $z = u_z$.

Several kinetic models can be found in the literature. In this paper, the kinetic cure reaction is modeled using an empirical rate expression [6] for the epoxy resin:

$$R_a = \left(Ae^{\left(\frac{-E_a}{RT}\right)}\right) (1-\alpha)^n \tag{3}$$

where A is the frequency factor, n is the reaction order, R is the universal ideal gas constant, E_a is the activation energy and α is the degree of cure.

The fiber-resin system was assumed to be epoxy resin and glass fiber. The physical properties of the composite were calculated by the following equations [1]:

$$\rho_{\rm c} = \phi_r \, \rho_r + \phi_f \, \rho_f \tag{4}$$

$$\rho_c C_{p_c} = \rho_r \phi_r C_{p_c} + \rho_f \phi_f C_{p_f}$$
(5)

$$\frac{1}{k_c} = \phi_r \frac{1}{k_r} + \phi_f \frac{1}{k_f} \tag{6}$$

where the subscripts r, f and c represent resin, fiber and composite respectively.

Table 1 presents approximated data from literature (Santiago et al., 2003) about physical properties and cure kinetics, respectively, of epoxy resin and glass fiber used in this paper.

Table	1.	Physical	Properties	and	Kinetic	Parameters	(Santiago
et al.,	20	03)					

Fiber fraction (Φ)	0.85		
Density of the resin (ρ_r)	1234 (kg/m ³)		
Density of the fiber (ρ_f)	2580 (kg/m ³)		
Thermal conductivity of the resin (k_r)	0.169 (J/m.s)		
Thermal conductivity of the fiber (k_f)	0.866 (J/m.s)		
Thermal capacity of the resin (Cp_r)	1.833 (kJ/kg.K)		
Thermal capacity of the fiber (Cp_f)	0.833 (kJ/kg.K)		
Initial temperature (T_0)	300 K		
Initial concentration of resin (Ca_0)	1100 (kg/m ³)		
Frequency Factor (A)	2.918x10 ⁶ (s ⁻¹)		
Activation Energy (E_{a1})	1.07x10 ⁵ (kJ/kg)		
Order of reaction (n)	2		
Universal constant of gases (R)	8.33 (J/mol K)		

3.2. Initial and boundary conditions

The degree of cure is considered zero, $\alpha = 0$, at the die entrance and the initial temperature of the system is T_0 .

Because of the symmetry, the heat flux in the composite center of the composite is equal to zero.

Thus
$$\frac{\partial T}{\partial r}\Big|_{r=0} = 0$$
.

The die surface, r = R, may be adiabatic or not. Both cases were studied in this paper. In the case of adiabatic die, the boundary condition is $q_s = 0$.

When the die is not adiabatic, the boundary condition is described by the convective heat flux, $q_s = h(T_s - T_a)$ where h is the convective coefficient, T_s is the die surface temperature and T_a is the environment temperature.

3.3. CFD method

For the numerical solution, it was used a CFDtype model. Computational Fluid Dynamics (CFD) is a computer-based tool for simulating the behavior of systems involving fluid flow, heat transfer, and other related physical processes. Fluid flow equations are solved over a region of interest with specified conditions on the boundary of that region. The numerical method on which ANSYS CFX 11.0[®] is based is known as the finite volume technique. In this technique, the region of interest is divided into small sub-regions, called control volumes. The equations are discretized and solved iteratively for each control volume. As a result, an approximation of each variable value at specific points throughout the domain can be obtained. Each node is surrounded by a set of surfaces that define the control volume. All the solution variables and fluid properties are stored at the element nodes.

4. METHODOLOGY

Two different heater arrangements were proposed herein: heaters on the die surface - the most usual heater arrangement proposed in literature – and heaters inside an insulated die. Next, these arrangements are explained.

4.1. Heaters on the die surface

It was used a steel die of 1 m in length with transversal area of 0.16 m^2 . Six rectangular electrical heaters, with dimensions of $0.04 \text{ m} \times 0.2 \text{ m}$, coupled on die surface and spaced of 0.1 m, were used. The composite has 0,006 m in radius and the same length of the die. A half of this die tooling is shown in figure 2. A convective heat coefficient of $10 \text{ W/m}^2 \text{ °C}$ was used to model heat transfer between the outer

die surfaces and the surrounding air, which was assumed to be 298K, normally used in the reported literature (Meyer, 1985; Santiago et al, 2003). Using symmetry, only a quarter of the pultrusion tool was considered in the numerical model. A volume mesh consisted of 99,860 nodes and 410,052 elements, was sufficient to simulate the process.



Fig. 2. Heaters on the die surface.

4.2. Heaters inside an insulated die

For this, it was suggested a new tooling pultrusion die consisted of internal heaters inside an insulated die. The material and their properties were the same considered before. The distance between each heater was set to be 0,2 m. The dimensions were reduced comparing with the configuration before. It was assumed the dimensions of 0.002 m x 0.002 x 0.06 m. This heater arrangement can be seen in figure 3. The number of nodes sufficient to the simulation was 110,726 and the number of elements was 550,069.



Fig. 3. Internal heating in an insulated die.

F

The goal is to minimize the process energy rate, which is written by a linear objective-function, subjected by a non-linear constraint. The objective function is written as the energy rate of the process:

$$= q_h + P(\alpha, \xi) \tag{7}$$

where:

 $P(\alpha,\xi) = \xi \cdot \max[g(\alpha),0]^2$ is a penalty term that incorporates the following constraint:

$$g(\alpha) = \alpha_{min} - \alpha, \qquad (8)$$

in which ξ is a penalty factor, and α_{min} is the minimum degree of cure to be reached. $g(\alpha)$ is the difference between the minimum value of cure degree to be reached at die exit and the degree of cure at this point. For the minimization of energy rate it was developed a FORTRAN code that links CFD with a particle swarm optimization (PSO) algorithm (Kennedy & Eberhart, 1995) to optimize it. PSO allows a global minimization in a predefined search region, without the need of initialization parameter guesses and without differentiation of the objective function. This algorithm may optimize a problem by maintaining a population of candidate solutions called particles and moving these particles around in the searchspace according to a simple formula. The movements of the particles are guided by the best found positions in the domain region, which are continually being updated as better positions are found by the particles.

5. RESULTS AND DISCUSSION

5.1. Heaters on the die surface

The pultrusion process was optimized with use of a particle swarm optimization, assuming different values of heat flux at each heater, until finding a minimum value of energy consumption to cure the material, figure 4. Assuming this heater arrangement, a heat flux equals to 25 kW.m^{-2} at the first heater (energy consumption of 200 W) was necessary to reach a degree of cure near the maximum value at the die exit. In this case, only the heater 1 was sufficient to cure the resin-fiber system and the others two heaters were not necessary to be used. In figure 5, it is possible to observe the increase of temperature near the first heater up to 537 K around the middle of the die the temperature stabilized in 500 K.

According to the reported literature (Basuki et al., 1998; Carlone et al., 2007; Coelho et al., 2002) the heat flux at the final stage of the cure reaction can be decreased due to the fact that the heat generated by the cure reaction inside the die can provide enough energy to cure the material at this stage. Hence, the temperature assumes different values along the die length and it may be reduced at the final stage of the cure. Considering this fact, the only way to reduce the energy consumption for this configuration is reducing the flux in heater 1. Therefore, it was assumed a value of 20 kW.m⁻² in heater 1. It can be noted in figure 6 that this value was not sufficient to totally cure the material. The degree of cure achieved only a value next to 0.9 at the die exit and the temperature achieved a value of approximately 490 K, as seen in figure 7.



Fig. 4. Degree of cure profiles: (a) at the composite center (r = 0) and (b) at the composite surface. Both figures assume a heat flux equals to 25 kW.m⁻² at the first heater (total energy consumption of 160 W).

5.2. Heaters inside an insulated die

The same procedure explained in section 5.1 was used here, in order to find a minimum value of energy consumption during the cure process. After several iterations of PSO algorithm the minimum energy consumption to obtain a degree of cure value near the maximum value was 270 kW.m². at the first heater and a heat flux of 8 kW.m⁻² at the second heater (total energy rate of 132 W), figure 8. As seen in figure 9, the temperature profile changed along the die length. It can be seen that the composite temperature, after approximately the die length of 0.4 m, was higher than the die wall temperature because of

the energy released by the exothermic cure reaction inside the die. Therefore, decreasing the temperature after this point was primordial to spend less thermal energy. The result obtained by using internal heating configuration was compared with experimental results obtained from Santiago et al. (2003). As seen in figure 10, the temperature distribution of experimental data is similar to obtained in our simulation.



Fig. 5. Temperature profiles: (a) at the composite center (r = 0) and (b) at the composite surface. Both figures assume a heat flux equals to 25 kW.m⁻² at the first heater (total energy consumption of 160 W).



Fig. 6. Degree of cure profiles: (a) at the composite center (r = 0) and (b) at the composite surface. Both figures assume a heat flux equals to 20 kW.m⁻² at the first heater (total energy consumption of 160 W).

It is observed that heaters with wide superficial area spend unnecessary energy to provide a desired value of temperature on a certain location of the die. It is clear that decreasing the area of heat transfer between the heater and the die, the same temperature value may be obtained consuming less thermal energy. Besides, heaters with smaller superficial area can provide a high degree of cure spending less thermal energy. The internal heating configuration using an insulated die spent 132 W, while rectangular heaters on the die wall spent 160W.

The maximum experimental temperature is higher than 500 K while the higher optimized temperature is approximately 480 K. The theoretical temperature profile in the center of composite presents a smoother distribution when compared with theoretical results.



Fig. 7. Temperature profiles: (a) at the composite center (r = 0) and (b) at the composite surface. Both figures assume a heat flux equals to 20 kW.m⁻² at the first heater (total energy consumption of 160 W).



Fig. 8. Degree of cure profiles: (a) at the composite center (r = 0) and (b) at the composite surface. Both figures assume a heat flux equals to 270 kW.m⁻² at the first internal heater and a heat flux of 8 kW.m⁻² at the second internal heater (total energy consumption of 132 W).



Fig. 9. Temperature profiles: (a) at the composite center (r = 0) and (b) at the composite surface. Both figures assume a heat flux equals to 270 kW.m⁻² at the first internal heater and a heat flux of 8 kW.m⁻² at the second internal heater (total energy consumption of 132 W).



Fig. 10. Temperature profiles: comparison with experimental results.

6. CONCLUSIONS

Governing equations for the resin flow during pultrusion have been modeled and a CFD method has been developed to solve the equations. In the pultrusion process, an optimum temperature profile was represented by a temperature distribution imposed on the die wall according to a kinetic cure reaction inside the die. A set of internal heaters inside an insulated pultrusion die was established successfully in order to achieve a composite part with a temperature of 440 K and a maximum degree of cure at the die exit.

This result shows it is possible to produce composite material in a more economical way if by changing thermal configuration, as the one suggested herein. Therefore, it is important to know the dimensions and configuration of heaters in order to configure the temperature profile.

The following conclusions can be drawn from the results presented in this paper:

- 1. The temperature profile depends strongly upon the heating configuration of the die assemble. Heaters with small transversal area must be primarily assumed to simulate the process. According to the results, heaters with wide transversal area may spend excessive thermal energy to cure the resin.
- 2. The suggestion of internal heaters in an insulated die may improve the thermal efficiency of the process avoiding the energy loss to the environment and it turns the die insulation easier.
- 3. The results suggest new studies about heater arrangements of the pultrusion process. Each particular case must be examined, taking account the variables and the geometry of the desired composite.

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STRATEGIA OPTYMALIZACJI DLA ZASTOSOWANIA KOMPUTEROWEJ DYNAMIKI PŁYNÓW DO PROCESU PRASOWANIA CIĄGŁEGO

Streszczenie

Prasowanie ciagłe jest procesem służącym do wytwarzania kompozytów, w którym włókna są przeciągane w sposób ciągły przez kąpiel z impregnatu z żywicy, a następnie podawane do podgrzewanej matrycy, w której następuje reakcja egzotermiczna powodująca polimeryzację. Energia cieplna niezbędna dla tej reakcji zależy od wielu czynników, takich jak kinetyka procesu i prędkość przeciągania. Sześć prostokątnych grzejników jest przeważnie umieszczanych na powierzchni matrycy aby nagrzać materiał. W niniejszej pracy wykazano, że moc potrzebna do zajścia reakcji może być znacznie ograniczona poprzez zmianę tego powszechnie stosowanego w praktyce układu grzejników. W zaproponowanej nowej konfiguracji zastosowano grzejniki wewnętrzne o mniejszej powierzchni. Nowy układ symulowano modelem wykorzystującym komputerową dynamikę płynów (ang. Computational Fluid Dynamics - CFD). Wyniki symulacji porównano z dostępnymi w literaturze pomiarami i wykazano, że zaproponowany układ grzejników umożliwia obróbkę materiału w sposób bardziej efektywny. Metoda roju cząstek została zastosowana do znalezienia minimum mocy.

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