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CFD-OPTIMIZATION ALGORITHM TO OPTIMIZE THE ENERGY TRANSPORT IN PULTRUDED POLYMER COMPOSITES

L. S. Santos[1*], E. C. Biscaia Jr.[2], R. L. Pagano[2] and V. M. A. Calado[1]

[1]Escola de Química, Universidade Federal do Rio de Janeiro, Rio de Janeiro - RJ, Brasil.
E-mail: lizandrosousa@yahoo.com.br
[2]Programa de Engenharia Química, COPPE, Universidade Federal do Rio de Janeiro - RJ, Brasil.

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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 into a heated die, where an exothermic cure reaction occurs. The energy needed to provide the cure reaction depends on many aspects such as cure kinetics and pulling speed. Generally, the pultrusion forming is divided in heat zones that can be heated at different temperature levels. The temperature distribution on the die surface can greatly affect material quality and energy cost. In the present work, through a CFD (Computational Fluid Dynamics) algorithm, it was possible to verify that the energy requirements can be reduced by changing the heating configuration of the pultrusion die. For this, an alternative configuration with internal heaters inside the die body was simulated. The heating rate was considered as the objective function. For the optimization study, we used a stochastic algorithm, the so-called particle swarm optimization (PSO) algorithm. The results showed that the energy spent to cure the resin-fiber system can be reduced considerably.

Keywords: Cure reaction; Computer fluid dynamics; Polymer composite; Particle Swarm.

INTRODUCTION

Composite materials can be used effectively for structural applications where high strength-to-weight and stiffness-to-weight ratios 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 of pulling continuous fibers 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*., 1998). The die can 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 where a cut-off saw cuts the parts to the desired length. Figure 1 shows a scheme of pultrusion equipment.

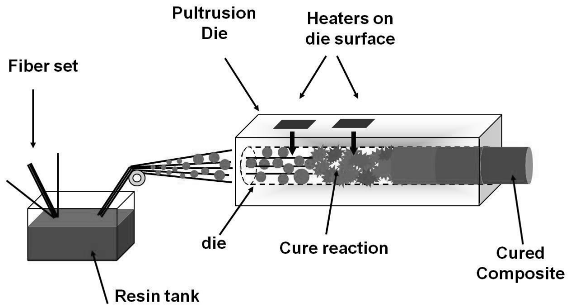

Figure 1: Pultrusion equipment.

The degree and uniformity of cure influence the

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*To whom correspondence should be addressed composite's mechanical properties. A non-uniform distribution of degree of cure over the cross section of the material implies a product of unreliable quality (Coelho and Calado, 2002). Variables such as the die temperature, pulling speed, pulling force and resin cure kinetics are important to control the process and to produce a material with high quality. 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 and Calado, 2002). Therefore, it is important to control the temperature distribution at each stage of the process without affecting the cure reaction.

PRIOR WORK ON SIMULATION AND OPTIMIZATION OF PULTRUSION

A number of researchers have solved the nonlinear differential equations that represent the physical phenomena of a pultrusion process. Han *et al*. (1986) were among the first researchers to simulate pultrusion. In their study, the finite difference method was applied to solve the model and the temperature distribution of the composite could be obtained. The influence of the reaction inside the die cavity on the temperature profiles could be explained according to the numerical results. Santiago *et al*. (1997) simulated the pultrusion process of a cylindrical composite by using the finite element method. The results for the temperature profile were very close to experimental ones. However, some aspects are incomplete in these works (Han *et al*., 1986 and Santiago *et al*., 1997) regarding the temperature profile imposed on the die wall: It was not clear what should be the equivalent heating arrangement of the pultrusion die.

Some researchers have simulated pultrusion by using finite element (FE) packages to perform heat-transfer and mass-transfer analyses. Moschiar *et al*. (1996) and Li *et al*. (2001) simulated the pultrusion process by using a die with three heat zones described by three heaters along the die length. Other researchers such as Srinivasagupta and Kardos (2003) optimized the pultrusion process based on a minimization of an objective function. Generally, this function represents the energy economy or process profit. Srinivasagupta and Kardos (2003) used a thermodynamic objective function to minimize the energy consumption during the cure reaction. These authors and Joshi *et al.* (2003) considered that the number and geometry of the heaters were previously known before the numerical optimization. All these authors (Moschiar *et al*., 1996; Li *et al*., 2001; Srinivasagupta and Kardos, 2004; Joshi *et al.,* 2003) 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 changes in the heating arrangement on the energy cost.

In the present investigation, a numerical procedure based on the finite element method was used to solve the mathematical model and a stochastic optimization algorithm was considered for the optimization study. Our strategy was to join the desirable characteristics of CFD tools and a particle swarm optimization (PSO) algorithm in order to produce an efficient optimization procedure. The goal was to minimize the process energy rate, which is written as a linear objective-function, subject to a non-linear constraint. In order to calculate this function, the algorithm solves the mathematical model inserted in the CFD package. This CFD-optimization technique had not been explored yet for the pultrusion process.

METHODOLOGY

According to the reported literature (Voorakaranam *et al*., 1998, Coelho and Calado, 2002) the heating rate at the final stage of the cure reaction can be decreased due to the fact that the thermal energy released inside the die by the cure reaction can be sufficient to cure the material at this stage. Hence, an optimal heat arrangement is strongly dependent on the cure kinetics.

We believe that the typical heater configuration, as suggested by Liu (2003), Figure 2, can be arranged in a more efficient way in order to avoid energy loss during the process. Therefore, we suggest an alternative die configuration with internal heaters, as seen in Figure 3. The aim of this heating policy is to increase the number of arrangement possibilities (decision variables). In this way, the algorithm is able to distribute the heat on the pultrusion die in a more efficient manner.

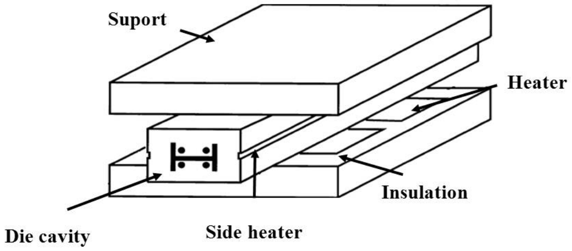

Figure 2: Pultrusion die studied by Liu (2003).

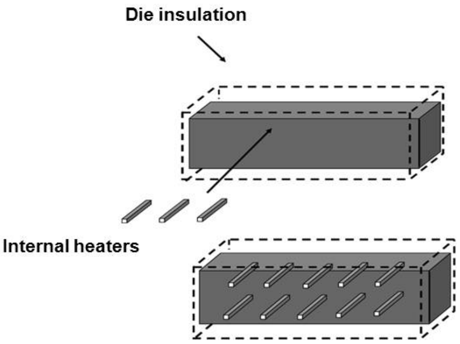

Figure 3: Internal heaters in a pultrusion die.

Heat transfer in the pultrusion process can be modeled using the energy equation and a cure reaction model. In this study, a steady-state condition was assumed and an "I beam" cross section composite profile, as seen in Figure 2. The three-dimensional energy balance of the composite part can be expressed as:

$$\rho_c \, Cp_c \left(u_i \cdot \nabla T\right) = k_c \nabla^2 T + Ca_o (1-\varphi_f) \Delta H_r r_a \qquad (1)$$

where the variation of degree of cure along the die length is expressed as:

$$\frac{d\alpha}{dt} = \frac{d\alpha}{dz} \cdot u_z = r_a \qquad (2)$$

where $u_z = z / t$ and therefore $dt = dz / u_z$.

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

$$r_a = \left(A e^{\left(\frac{-E_a}{RT}\right)} \right) (1-\alpha)^n \qquad (3)$$

The physical properties of the composite were calculated by the following equations (used by Santiago, 2003 and Liu, 2003):

$$\rho_c = \phi_r \rho_r + \phi_f \rho_f \qquad (4)$$

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

$$\frac{1}{k_c} = \phi_r \frac{1}{k_r} + \phi_f \frac{1}{k_f} \qquad (6)$$

The degree of cure is considered to be zero at the die entrance and the resin feed temperature of the system is the environment temperature:

$$T_{z=0} = T_0 \text{. and } \alpha_{z=0} = 0 \qquad (7)$$

Because of the symmetry, as shown in Figure 2, the heat flux in the regions of symmetry is defined as:

$$\nabla T = 0 \qquad (8)$$

and the die surface is adiabatic:

$$q_s = 0 \qquad (9)$$

The heat conduction from the heaters is the sum of the power of each heater.

$$\sum_{i=1}^{n} q_i = q_h \qquad (10)$$

Tables 1 and 2 shows data from the literature (Liu, 2003) on the cure kinetics and physical properties, respectively, of the epoxy resin and glass fiber used in this study.

Table 1: Kinetic parameters

Symbol	Name	Value	Unit
A	Pre-exponential factor	$2.92\text{x}10^6$	s^{-1}
E_a	Activation energy	$25.57\text{x}10^3$	$J \cdot mol^{-1}$
n	Order of reaction	2	
R	Universal Gas Constant	8.314	$J \cdot mol^{-1} \cdot K^{-1}$

Table 2: Physical properties

Symbol	Name	Value	Unit
ϕ_f	Fiber volume fraction	0.45	
ϕ_r	Resin volume fraction	0.55	
ρ_r	Resin specific mass	1100	$kg \cdot m^{-3}$
ρ_f	Fiber specific mass	2560	$kg \cdot m^{-3}$
k_r	Resin thermal conductivity	0.169	$J \cdot m^{-1} \cdot s^{-1}$
k_f	Fiber thermal conductivity	1.04	$J \cdot m^{-1} \cdot s^{-1}$
C_{pr}	Resin specific heat	1640	$J \cdot kg^{-1} \cdot K^{-1}$
C_{pf}	Fiber specific heat	640	$J \cdot kg^{-1} \cdot K^{-1}$
T_o	Feed temperature	300	K
Ca_o	Feed resin mass concentration	1100	$kg \cdot m^{-3}$
ΔH_r	Heat reaction	398.4	$J \cdot kg^{-1}$
u_z	Pull speed in z direction	0.005	$m \cdot s^{-1}$
T	Temperature		K
α	Degree of cure		
Z	Pull direction		

OPTIMIZATION PROCEDURE

The objective function is written as the energy rate of the process:

$$F = q_h + P(\alpha, \xi) \tag{11}$$

where:

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

$$g(\alpha) = \alpha_{min} - \alpha, \tag{12}$$

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 the die exit and the degree of cure at this point. For the minimization of the energy rate a FORTRAN code was developed that links CFD with a particle swarm optimization (PSO) algorithm (Kennedy and Eberhart, 1995) to optimize it. The complete code can be visualized in Santos (2009).

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 can optimize a problem by maintaining a population of candidate solutions called particles and moving these particles around in the search-space 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.

The PSO version used in this work was idealized by Kennedy (1998) and also used in a modified version by Schwaab (2005). It consists of introducing a new weight factor, w, in the original version proposed by the same authors.

$$v_{i,d}^{k_{int}+1} = w \cdot v_{i,d}^{k_{int}} + c_1 \cdot r_1 \cdot \left(p_{i,d}^{k_{int}} - x_{i,d}^{k_{int}}\right) + c_2 \cdot r_2 \cdot \left(p_{global,d}^{k_{int}} - x_{i,d}^{k_{int}}\right) \tag{13}$$

$$x_{i,d}^{k_{int}+1} = x_{i,d}^{k_{int}} + v_{i,d}^{k_{int}+1} \tag{14}$$

where k_{int} is the PSO iteration, d is the search direction, v is the particle velocity and x is the position relationed to the search space, c_1 and c_2 are positive constants called cognitive and social parameters respectively, r_1 and r_2 are random numbers that vary at each iteration within the interval $[0 \;\; 1]$, p_i is the best point of an individual particle i and p_{global} is the best value found. The choice of parameters c_1, c_2 and w depends on the problem formulation

The CFD package is ANSYS CFX©, based on a modified finite element method based on control volumes. In the proposed application, the polymer resin is considered to be a fluid that reacts and solidifies inside the die cavity. After integration of the pultrusion model, the temperature profile and degree of cure are the information that is used to evaluate the objective function. The flowsheet of our proposed optimization procedure is shown in Figure 4.

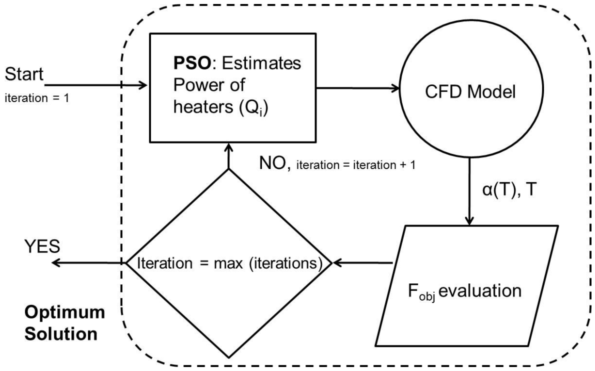

Figure 4: Optimization procedure.

RESULTS AND DISCUSSION

Theoretical Comparison with Results from Liu (2003)

In order to make a comparative study with results obtained in Liu (2003), two variables were analyzed: (a) the temperature profile of the composite center and (b) the cure profile at the composite center. The dimensions of the pultrusion die and composite are the same as those of Liu (2003). In Figure 5, the temperature profile presents a behavior similar to the profile obtained by that author. Both results indicate that the maximum value of the temperature is reached approximately between $z = 0.9$ and 1.0. After this location, the temperature decreases until reaching the die exit. This temperature peak occurs because of the energy rate released by cure reaction.

In this region, there is a large temperature gradient due to the kinetic behavior. This evidence can be checked in Figure 6, in which the cure profile is illustrated at the composite center. The result f shows that the cure gradient is strongly increased after $z = 0.8$. It is clear that, after this point, the composite part presents higher values of temperature and, consequently, the resin cures faster in this region. However, before this location, the resin presents a low kinetic rate and therefore the temperature decreases.

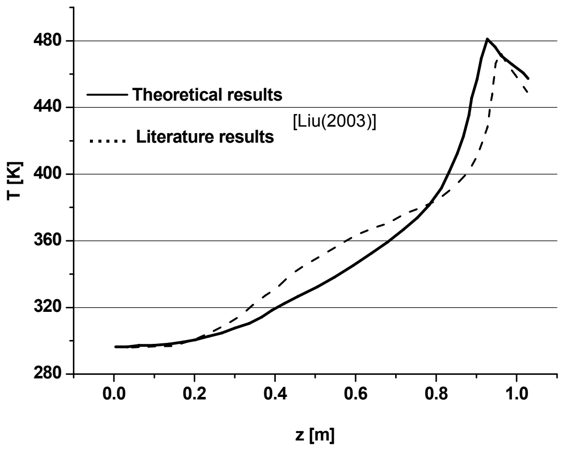

Figure 5: Temperature profile at the composite center.

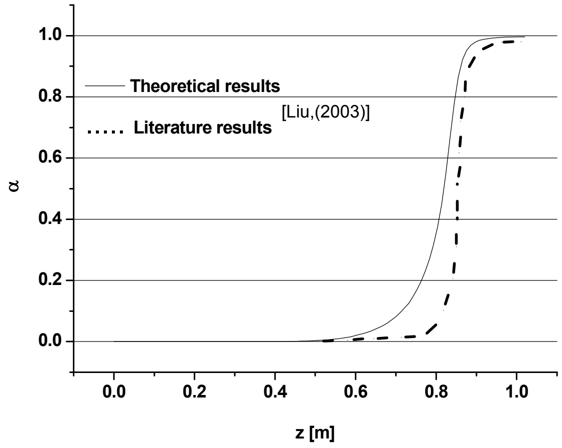

Figure 6: Cure profile at the composite center.

The results of Figures 5 and 6 show that the numerical results have an expected behavior in accordance with the thermal-kinetic behavior of the pultrusion process. The acceptance of these numerical results implies that the proposed model is capable of simulating this process according to theory expectations. Therefore, this model was used for the optimization study.

Optimization Study

In this topic we show the optimization of the case-study previously presented. Here, a modified pultrusion die with smaller internal heaters coupled inside was proposed, as seen in Figure 3. This choice increases the number of decision variables. The optimization algorithm was then applied to this new die arrangement in order to cure the material at a minimum of 95% of the rate of conversion.

The optimization results are shown in Table 3. At each iteration the algorithm estimates different values of the heat flux for each individual heater in order to find the optimal solution. As shown in Table 3, the optimization algorithm estimates five values of the heat flux that correspond to the five heaters coupled in the pultrusion die. The total energy rate and degree of cure at the die exit are shown for each iteration. According to the results, after three iterations of PSO, the minimal energy rate found was 260 W, corresponding to that average minimal energy rate used to cure the resin to a degree of 95%. It is clear that the algorithm reduced the power of the last heater near the die exit. This is due to the fact that, in this region, the die is sufficiently heated because of the heat released from the cure reaction. Another point to be checked is the number of iterations of the optimization algorithm. As we see, only three iterations were necessary for convergence. After that, no better results were found. This behavior can be explained by the following fact: the optimization algorithm is a particle swarm that presents a stochastic nature. In order to solve this problem, we chose 40 particles, which is sufficient to find a good result, possibly the optimal result, and requires few iterations. In this pultrusion problem, the maximum number of iterations was set to 10, but after the third one the PSO was not able to find an energy rate smaller than 260 W.

Table 3: Optimization results

PSO Iteration	q_1 $\left(W \times m^{-2}\right)$	q_2 $\left(W \times m^{-2}\right)$	q_3 $\left(W \times m^{-2}\right)$	q_4 $\left(W \times m^{-2}\right)$	q_5 q_5 $\left(W \times m^{-2}\right)$	Energy rate (W)	Degree of cure at composite center
1	16324	28595	11799	20974	201	389	0.98
2	12834	12333	11370	8139	7512	272	0.96
3	12828	12333	11370	8117	7512	260	0.95

In order to compare these results with the results of Liu (2003), the temperature profiles at the composite center were plotted. Figure 7 shows the temperature profile obtained from the optimization procedure, which shows very similar behavior to that reported by Liu *et al*. (2003. This would appear to be a contradictory result because the energy rate is theoretically smaller in this optimal case. However, the energy rate used to heat the material is distributed on the die body in a more efficient way, yet presents a similar temperature profile at the composite center. Figure 8 shows the temperature profile at other points of the composite section. It is clear that there are locations where the temperature is higher than the value of 460 K achieved at the composite center, the result of a high gradient of temperature inside the composite. In the same way, Figure 9 depicts the degree of cure profile. The material cures first at the center, achieving the maximal value near to the die exit region. This result shows that the material cures along all the die length, in contrast with the non-optimal results, in which the material cures only near the die exit as shown in Figure 6.

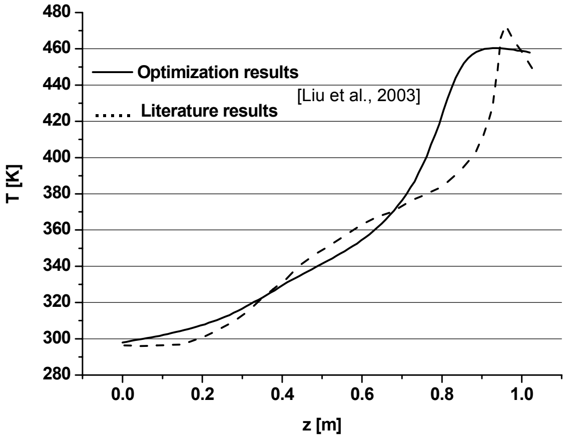

Figure 7: Temperature profile at the composite center (compare to Figure 5).

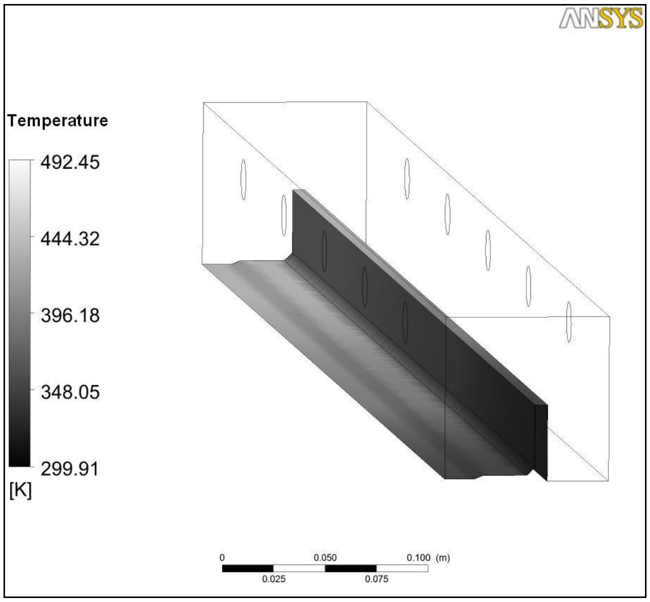

Figure 8: Temperature profile of the composite part.

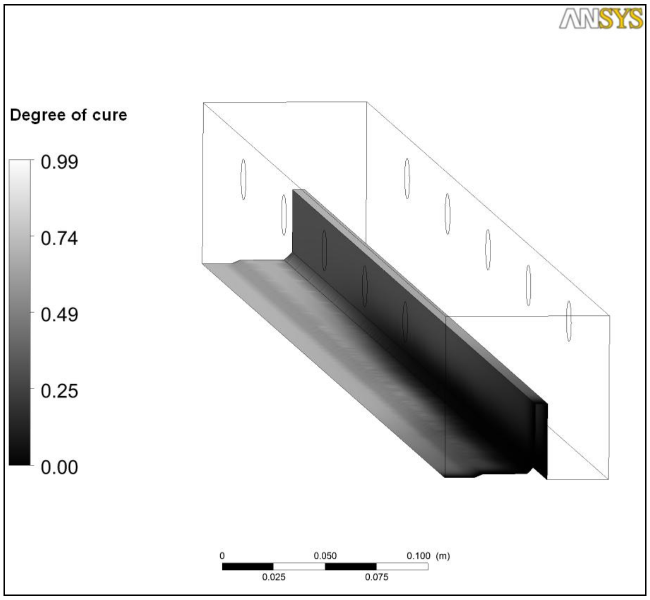

Figure 9: Cure profile of the composite part.

CONCLUSIONS

The pultrusion model could be solved by a CFD package, resulting in a good prediction of temperature and degree of cure profiles. This routine, together with an optimization algorithm, is successful in optimizing the pultrusion problem. In our case, we used the PSO algorithm, which was able to find the best operational point, by minimizing the total energy rate. The algorithm tends to reduce the temperature, mainly in regions where there is a high gradient of temperature due to the cure reaction.

Another contribution of this work is the link between CFD codes and external optimization routines. Here we made use of a PSO routine, but other options could be used with the present software. Particularly in pultrusion optimization it proved to be a relevant tool when the aim was to use CFD software in order to model the pultrusion process of composites with different geometries and die configurations.

The suggestion of internal heaters can increase thermal efficiency of the process by improving the thermal distribution on the die body. This heating arrangement also allows insulating the die surface.

The results suggest new studies of heater arrangements in the pultrusion process. Each particular case must be examined, taking into account the variables, heater positions and the geometry of the desired composite.

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