NUMERICAL SIMULATIONS OF METAL ONTO COMPOSITES CASTING

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ABSTRACT

The current paper presents a general three dimensional finite element model for modelling thermal degradation of polymer composites due to thermal loading. In particular, the model is intended for modelling the thermal degradation of polymer composites due to overcasting with light alloy metals. In this work, the model is implemented and solved using the general purpose FE-package Abaqus 6.7. The applicability of the code to more complex geometries was demonstrated by analysing the casting process of a metal ring onto a composite axle, resulting in a shrinkage fit. To succeed in manufacturing of this type of joint, a delicate balance between thermal loadings, metal shrinkage, composite degradation and the overall cooling must be met. The proposed subroutine together with FE-models provides the spatial distribution of these field variables, allowing for subsequent optimization of the shrinkage fit. In addition to the results presented here proper boundary conditions and material properties affected by the remaining resin content and more accurate modelling including effects from gas transport and cooling have to be included in the FE-analysis. This will be the subject for the continuation of this project.

KEYWORDS: Metal casting, multi-materials, thermal degradation, FEM

1. INTRODUCTION

The technical community of today is making increasing demands on weight reduction mainly for energy savings, particularly in the automotive industry, but also for better product ergonomics, for instance in the power tools sector. A lightweight product is usually produced using lightweight materials, for instance by integrating composites components into classical metal structures. This approach results in a complex multi-material product, where a number of different materials are combined in one component.

One of the biggest challenges in producing complex multi-material products is the need of joining the different materials together. Today, such products are usually produced by the means of mechanical or adhesive joints. Unfortunately, all of the current joining techniques results in a number of difficulties. For instance, the mechanical joints are often heavy while the adhesive joints are time-consuming to produce and therefore expensive.

In the present work, an alternative method of joining metal and composites is considered. In this method a thin metal layer is cast directly onto the composite component. Provided that the exposure time at high temperature is short enough, the polymeric material will not decompose considerably while the metal solidifies [1]. The joint is then formed either by geometric features, locking the two parts together, or by shrinkage fit (assuming that the metal is cast around the composite component). An example of a metal onto composite part is presented in Fig. 1 where a carbon fibre/epoxy (CF/EP) rod is joined to a pressure die casted aluminium component.

Fig. 1. Composite rod imbedded in pressure die casted aluminium.

The method of overcasting has potential to eliminate a number of production steps and in consequence reduce manufacturing time and therefore cost. However, the process itself is very complex and thus difficult to understand. Therefore, development of new products would require extensive and costly testing. For that reason it is attractive to replace some of the tests by numerical simulations.

During the casting of melted metal onto composites, thermal degradation of the polymer will occur. Given that the exposure time is short and temperature sufficiently low this degradation may be kept to a minimum. There exist several one-dimensional models that describe the thermal process of degrading polymers [2-6]. However, to account for multi-dimensionality of a real product, these models have to be developed further and solved using numerical methods. A predictive and validated model for the thermal response of composite materials will help to minimize the number of tests required for development of new products. Realistic thermal degradation modelling will provide the designer with the capability to demonstrate innovative, new designs using the bespoken overcasting technology, which will minimize the initial resources and expensive testing.

The aim of this work is, therefore, to utilize a general three-dimensional finite element model to simulate the overcasting process of metal onto composites parts. While the finite element model permits a general representation of the decomposition process and different boundary conditions, the specific constitutive decomposition model presented here is based on a first-order Arrhenius equation with constant thermal and transport properties throughout the decomposition process. The decomposition model has been implemented as a subroutine to the commercial software Abaqus 6.7 in the FEM-modelling procedure. The accuracy of the model has been evaluated by comparing the predicted temperature profiles with those obtained from the verified code COM_FIRE version 4.0 [7]. Having said that, it should be emphasized that the results presented in this paper are part of an ongoing project, and as such, they may be subjected to changes in a future analysis. Especially when a more precise modelling considering temperature/degradation dependent specific heat capacity and thermal conductivity in conjunction with the gas cooling effect will be performed. Nevertheless, we firmly believe that the thermal modelling presented herein have helped to improve the understanding of the overcasting process.

2. THEORETICAL BACKGROUND

There are several mathematical models that have been developed which simulate the thermal response of materials undergoing decomposition and chemical reactions and basically they are all similar in principle. Usually they are based on heat conduction through the thickness of the structure including thermal effects of the organic material decomposition (the decomposition of organic substances is an endothermic process which has a temporarily delaying effect of the transmission of heat through the structure). To account for this temperature-dependent thermal decomposition an *n*-th order Arrhenius equation is normally utilized [5]. Following the work by Looyeh et al. [4] which is based on the model originally proposed by Henderson et al. [2] the phenomenon of energy conservation for heat transfer in a material undergoing thermal decomposition is given by the non-linear partial differential equation:**x**

$$\rho C_p \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial \mathbf{x}^2} - \frac{\partial \rho}{\partial t}\left(Q_d + h_c - h_g\right) \tag{1}$$

where bold face indicate a tensorial field variable. Q_d is the heat of decomposition. h_c is the enthalpy of the composite and h_g the generated gas enthalpy. In addition to the assumptions made in their model, a further simplifying assumption here is that the heat exchange between the decomposing composite and the decomposition gas transported through it is disregarded. For a fibre reinforced composite with aligned long or continuous reinforcement, the density ρ and specific heat C_p are evaluated by the rule of mixtures as:

$$\rho_c = \rho_f \phi + \rho_m (1-\phi) \tag{2}$$

$$C_p^c = \frac{C_p^f \rho_f \phi + C_p^m \rho_m (1-\phi)}{\rho_c} \tag{3}$$

ϕ is fibre volume fraction and indices f and m stands for fibre and matrix respectively. Instead of using rule of mixtures the transverse thermal conductivity k_c of the composite may be more accurately determined from the conductivities of the fibre and matrix components using the well known Halpin-Tsai model

$$k_c = k_m \left(\frac{1+\xi\phi\eta}{1-\eta\phi} \right) \tag{4}$$

where

$$\eta = \frac{k_f / k_m - 1}{k_f / k_m + \xi} \tag{5}$$

ξ is a fitting parameter, but for fibres with circular cross-section $\xi = 1$ can be assumed. The enthalpy of the composites and the generated gas enthalpy have been assumed to be functions of temperature only and are given by:

$$h_c = \int_{T_0}^{T} C_p^c dT \qquad (6)$$

and:

$$h_g = \int_{T_0}^{T} C_p^g dT \qquad (7)$$

respectively. With the simplifying assumptions that the thermal and transport properties in the composite are constant during the decomposition these two equations become:

$$h_c = C_p^c (T - T_0) \qquad (8)$$

and

$$h_g = C_p^g (T - T_0) \qquad (9)$$

Both density and its loss rate are calculated by the Arrhenius equation

$$\frac{\partial \rho}{\partial t} = -A\rho_0 \left(\frac{\rho - \rho_f}{\rho_0} \right)^n e^{(-E/RT)} \qquad (10)$$

Indices *f* and *0* indicate final- and initial density respectively. *A* is the pre-exponential factor, *E* is the activation energy of decomposition, *R* is the gas constant and *T* is temperature. Application of this model requires knowledge of the kinetic parameters *A*, *E* and *n* of the resin which generally are acquired through thermogravimetric analysis (TGA). The set of equations (1, 8-10) has been implemented into a general FE-code: Abaqus 6.7 as a user subroutine.

3. EXPERIMENTAL RESULTS

In order to elucidate the degradation behaviour, and provide data for the thermal degradation process modelling, TGA experiments were performed in nitrogen atmosphere over temperatures ranging from 50 to 850°C using a Perkin-Elmer TGA-7 thermogravimetric analyzer. Runs were conducted at high heating rates of 100 °C/min on a standard EXEL epoxy resin system. Then following the work by Looyeh et al. [4] the endothermic decomposition of the resin may be described by a single thermally activated process using an *n*-th order Arrhenius equation assuming no expansion of the composite material:

$$\frac{\partial \rho}{\partial t} = \frac{\partial m}{\partial t} = -Am_0 \left(\frac{m - m_f}{m_0} \right)^n e^{(-E/RT)} \qquad (11)$$

where *m* is the mass of the resin. There are several approximate techniques using different approaches available for estimation of the kinetic parameters *A* and *E* from TGA measurements, e.g. the Coats-Redfern method, Ozawa method and Horowitz-Metzger method just to mention a few. In this paper however, the direct non-linear regression method explained by Slovak [8] have been utilized. This is a straightforward way of determining the kinetic parameters and may be conveniently implemented in any numerical computing environment, such as MATLAB for instance. The basic idea is first to replace the derivatives in Eq. (11) by finite differences. This is reasonable if the time step is chosen small enough and if we assume that the TGA curve is composed of very small linear segments in which the reaction rate is constant. Then Eq. (11) turns into the following recurrence relation:

$$m_i = m_{i-1} - Am_0 \left(\frac{m_{i-1} - m_f}{m_0} \right)^n e^{\left(-E/RT_{i-1}\right)} \left(t_i - t_{i-1}\right) \tag{12}$$

Slovak also expanded Eq. (12) for allowing to deal with several parallel processes. Here it is assumed that a single thermally activated process will suffice to describe the decomposition behaviour of the epoxy resin. Therefore, no expansion of expression (12) is necessary and the complexity of the Abaqus subroutine programming will be kept lower. The parameters *A* and *E* are determined by direct testing and screening of suitable values through a range of values with chosen accuracy. For each combination of *A* and *E* the residual sum of squares (RSS) is calculated comparing theoretically determined masses in individual points to the corresponding experimental points. The *A* and *E* combination giving the minimum RSS is then regarded as the best fit. Fig. 2 shows TGA curves at a constant heating rate of 100 °C/sec for two epoxy specimens and their average fitted curve using the first order Arrhenius expression (n = 1).

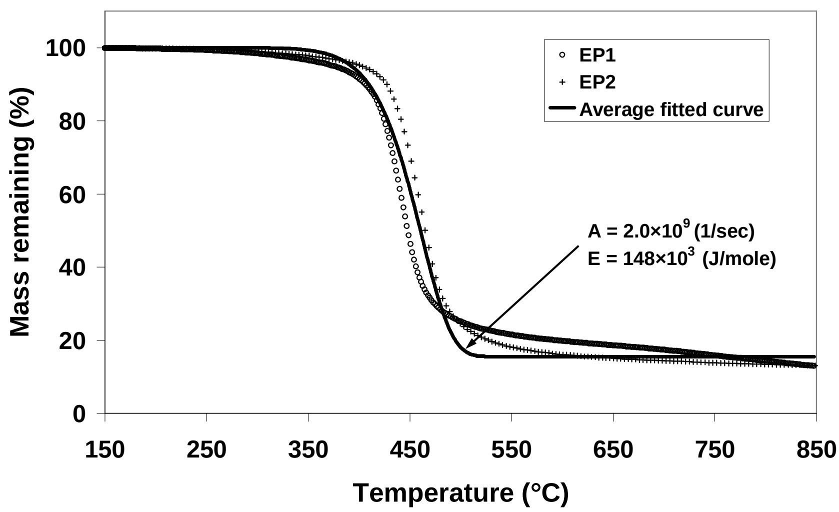

Fig. 2. TGA-curves for two epoxy specimens and their average fitted curve.

It is evident from Fig. 2 that a single thermally activated process using the first order Arrhenius equation does not give a perfect fit to experimental data in this case. The model cannot capture the behaviour of the curves in the beginning and in the end of the decomposition. This also addresses an important issue when dealing with modelling of the thermal degradation of thermoset polymers. Because there is no clear physical meaning of the kinetic parameters and the reaction order of a thermal degradation process for thermoset resins. The thermal degradation is attributed both to the gaseous products emission and to the chemical scission of the network bonding without gas emission and polymer weight loss [9]. Several processes can be operating at the same time, each having its own kinetic parameters. Therefore the kinetic parameters obtained here should be regarded as "apparent" values for these parallel processes.

4. NUMERICAL RESULTS AND DISCUSSION

4.1. Abaqus subroutine programming and validation against COM_FIRE

The commercial FE-program Abaqus 6.7 have been used in conjunction with user defined subroutines written in Fortran-code in order to model the thermal degradation problem. The subroutine USDFLD is used to calculate the remaining resin content (RRC) and redefine a field variable representing RRC which sets the density of the composite through the "dependencies" command in the Abaqus input file. Here it is assumed that the density of the laminate follows a linear relationship between the virgin material and the fully degraded material. The subroutine HETVAL is used to account for heat of decomposition and enthalpy change due to degradation. The accuracy of the programmed subroutine has been evaluated by comparing the predicted temperature profile and RRC of a degrading material with values obtained from the verified code COM_FIRE. The studied case was a 1-D problem using typical properties for a glass fibre vinyl-ester (GF/VE) laminate with $V_f = 0.6$. The geometry was 0.5 mm in height and 25 mm in thickness. 50 4-node linear diffusive heat transfer elements (DC2D4) were used through the thickness. The model was first checked against calculations in Excel assuming adiabatic and isothermal conditions, respectively. Then followed a comparison to COM_FIRE where the initial condition was set to 20 °C in the whole composite. A constant temperature of 700 °C was applied at one end and all other boundaries were insulated. Results obtained using Abaqus seem to be in accordance to those obtained with COM_FIRE, as can be seen in Fig. 3. There is a slight temperature difference, but the RRC shows a very good match.

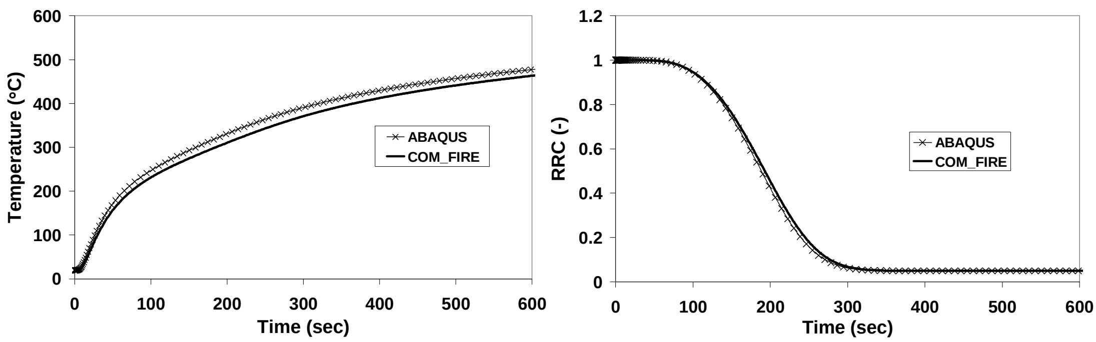

Fig. 3. Temperature variation and RRC for the GF/VE laminate 5 mm from the heated end.

The accuracy of the model has also been verified against COM_FIRE using two different models in 1-D case (not shown here): with and without gas transport and cooling. The comparison revealed a relatively small difference between the two cases.

4.2. FE-analysis of a CF/EP rod in cast aluminium

After verification of the subroutine in 1-D case a CF/EP composite rod was modelled using axisymmetric (DCAX4) elements. The material properties used in the modelling procedure are shown in Table 1. The values for density, specific heat and transverse thermal conductivity for the laminate were calculated using Eq. (2-4). The heat of decomposition Q_d which is also needed in the modelling is assumed to be 234 kJ/kg based on a value presented in literature [2]. However, it is pointed out that heat transmission through the composite is rather sensitive to this (in our case) unknown assumed parameter.

Table 1. Assumed material properties for the CF/EP laminate

Material	ρ_0 [kg/m^3]	k [W/mK]	C_p [J/kgK]	C_{pg} [J/kgK]	RRC_f [-]
Carbon fibre	1760	8.0	710	-	-
Epoxy resin	1250	0.3	1850	2400	0.155
Laminate	1556	1.05	1076	2400	0.155

In the following simulation a number of simplifications have been made, i.e. specific heat is assumed to be constant throughout the analysis whereas it is actually known to vary with both temperature and amount of degraded material. Thermal conductivity is assumed to be unaffected by temperature increase and level of degradation. In reality a porous char layer will form on the composite surface and act as an insulator. Here the carbon fibres are also assumed to be inert, whereas being an organic material, they too are prone to degrade at high temperatures. Furthermore, the composite is modelled as an isotropic material having only one value for thermal conductivity. A more thorough analysis should also include the anisotropic nature of the material and thus allowing for at least two values for thermal conductivities (transversely isotropic). In the continuation of this ongoing project these issues will be addressed in a more precise modelling procedure.

The composite rod surrounded by cast aluminium and the applied boundary conditions on the axisymmetric FE-modelled part is illustrated by Fig. 4. In the analysis 40 elements in thickness (radial) direction was used. The temperature variation on the composite boundary has been modelled earlier [1]. Here the nodal temperature on the surface of the rod was constrained to follow the temperature profile of the aluminium shown in Fig. 4. This implies very efficient heat transfer between the aluminium and the composite, which probably is more efficient than in reality. In order to later on improve the model the heat transfer between the aluminium and composite will be modelled using a convection boundary condition with a tailored convection film coefficient. Fig. 4 shows that the temperature profile on the composite boundary quickly declines from 760 °C down to about 110 °C in no more than five seconds. Obviously this behaviour will be related to the thickness of the aluminium overcasting component and the steel casting mould.

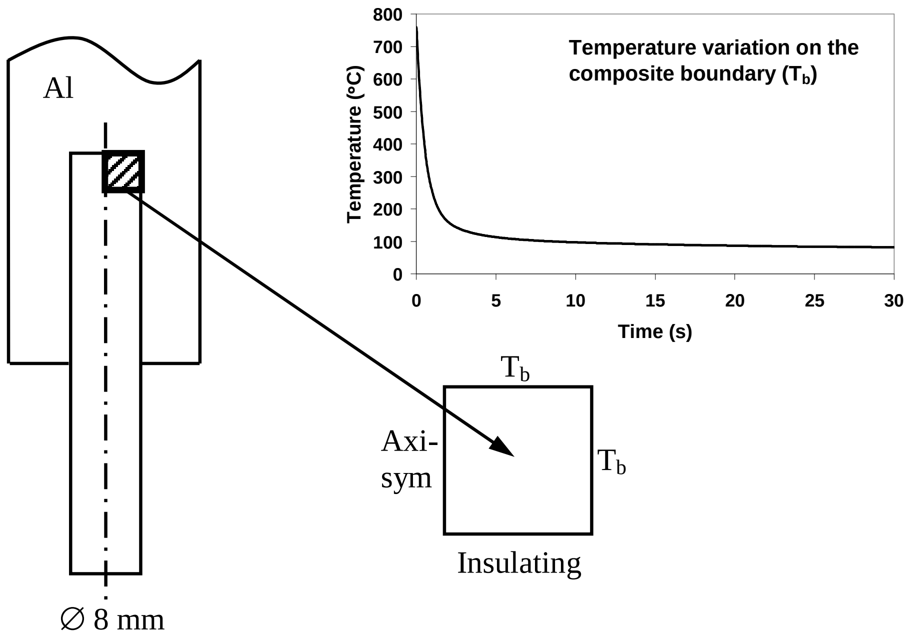

Fig. 4. Illustration showing the composite rod surrounded by cast aluminium and the FE-modelled part with boundary conditions.

The results of the simulation can be seen in Fig. 5-7. Fig. 5 and 6 shows temperature and RRC of the upper right corner of the axisymmetric modelled part respectively. In these figures the horizontal view is over the whole radius (4 mm).

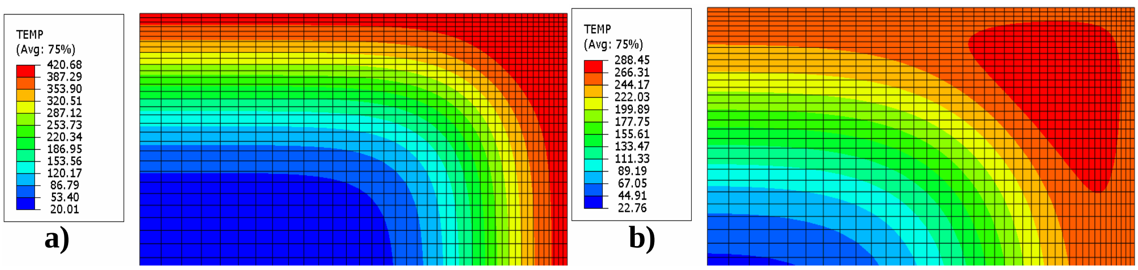

Fig. 5. (a) Temperature distribution in the composite after 0.5 sec and (b) after 1 sec.

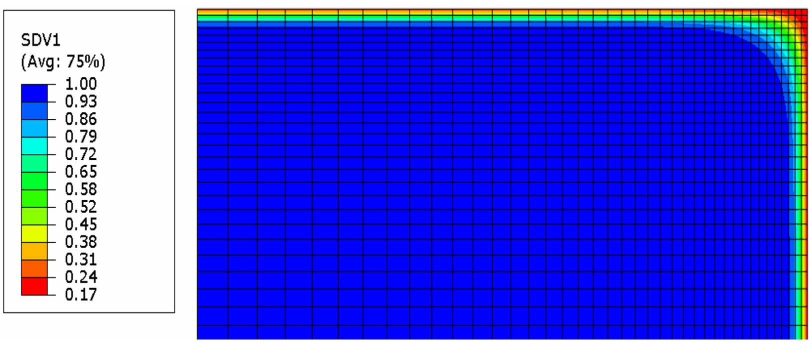

Fig. 6. RRC distribution in the composite after 30 sec.

It is evident from Fig. 6 that due to the relatively short exposure time only a small portion of the composite will be thermally degraded. The most critical part will be the corner and therefore, Fig. 7 shows RRC and temperature distribution along a 1 mm path drawn diagonally down from the upper right corner. It is concluded that approximately 0.8 mm along this path the material integrity will be totally unaffected by the applied thermal load. Further it can be seen that the temperature wave is travelling very fast through the material. After only 0.5 seconds at 1 mm along the path the temperature is about 345 °C. However, this is not totally unexpected due to the rather crude assumptions regarding the thermal properties of the composite/Al interface as mentioned earlier.

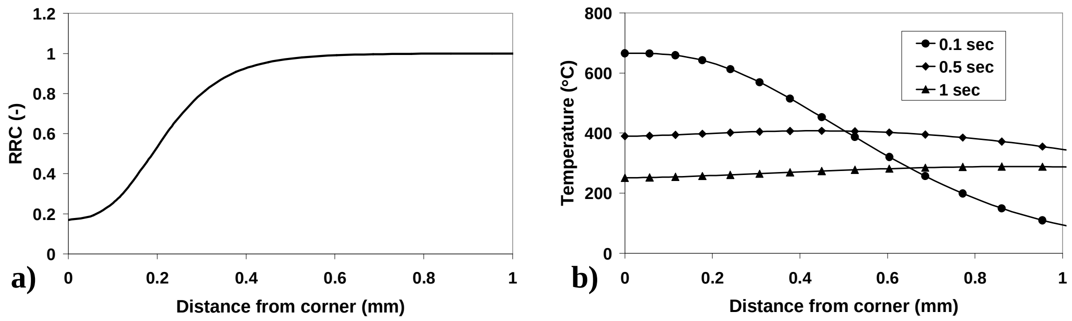

Fig. 7. (a) Final RRC (after 30 sec) and (b) temperature distribution along the diagonal path for three different time instants.

5. CONCLUSIONS

Modelling the thermal degradation of composites used for metal overcasting has two major benefits. First, it speeds up the design process and, thereby, reduces the cost of using this kind of manufacturing process. Second, it improves the knowledge of how these materials behave when exposed to elevated temperatures during overcasting.

The objective of this work was to develop and investigate the applicability of the finite element method to analyse the thermal behaviour of polymer composite materials when exposed to metal melt. Basic concepts of the phenomena occurring in the material exposed to the melted metal were described. The applicability of user defined subroutines developed during this study in conjunction with the commercial finite element program Abaqus 6.7 was demonstrated for thermal response of an axisymmetric composite component overcasted with aluminium. The model was verified against Excel calculations and the validated code COM_FIRE. The predicted temperatures and degree of degradation were found to agree well with the results obtained using COM_FIRE. The accuracy of the model was also verified against COM_FIRE using two different models in 1-D case: with and without gas transport and cooling. The comparison reveals a relatively small difference between the two cases. We therefore conclude that the proposed FE-model is able to simulate metal overcasting for a large range of typical composites components. As a result, this will allow for predictions of the shrinkage fit for these components and in consequence their mechanical performance. However, it is emphasized that the FE-model have to be validated against casting experiments and factors important for the overcasting process, such as proper boundary conditions between the aluminium and the composite, and material properties affected by the remaining resin content have to be included in the FE-model. The key factors are those that determine heat transmission through the protecting char layer, namely the endothermic decomposition effect, mentioned earlier, assisted by the low thermal conductivity of the fibrous reinforcement after the resin has been removed.

Finally, by using the finite element method, a wide range of geometries of composite components may conveniently be studied with little change to the subroutine computer code. Work on a more accurate three-dimensional model including effects from gas transport and cooling is ongoing.

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