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A Numerical Simulation of Cure Process Using General Coordinates Method

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Abstract

In this paper, a general coordinate control volume formulation for two-dimensional cure simulation of composite structures is introduced and a two-dimensional code is developed based on this formulation. In contrast to other numerical procedures based on the finite difference method, the present general coordinate method can easily model composite structures with arbitrary shapes. Results from the present cure simulations agreed well with the measured cure-induced temperatures and the numerical results from other experimental simulations.

Keywords: Cure simulation, control volume method, general coordinates, numerical code.

Introduction

Due to their strength ratios and high specific stiffness, composite materials are increasingly adopted for many applications and the demand for composite materials is extended to the construction of all kinds of structures. In fact thermosetting polymers are an important class of materials that have achieved widespread utilization in many high tech applications. The key advantage in the use of thermosetting polymers lies in the ability to start with a low viscosity liquid prior to curing, which allows us to tailor a specific material with our own desired characteristics.

These unique thermosetting specifications can be obtained by the curing mechanism which includes the chemical reactions that control both the chemorheology prior to gelation point followed by development of a highly cross linked network at full cure. The most important thermoset property is the degree of cure, which requires consistently high values (about 1.0 at full cure) to achieve the desired end-use physical properties.

According to *Min Li et al.* [1] autoclave curing is a process to produce fiber-reinforced polymeric parts in final shape. The simulation and optimization of autoclave processing have seen widespread application in industry as a means to understand and improve product quality. During processing, the autoclave is heated according to a predetermined temperature cycle and, at the same time, pressurized according to a predetermined pressure cycle. The applied heat increases the temperature in the composite, resulting in changes in the molecular structure of the resin and, correspondingly, in resin viscosity. When the resin viscosity has become sufficiently low, the applied pressure squeezes excess resin from the composite into a bleeder ply as the laminate consolidates. The resin then cures and cross-links, producing a rigid finished part.

If we are to describe some of the expressions used in the curing process of composites, we can include what *Sastry* [2] has mentioned: Impregnation describes the flow of resin into fiber rows; Consolidation describes the seamless compaction of laminate through interplay flow of resin, which both are required in processing. Tailoring of process cycles to achieve adequate degree of cure (thermosets) or degree of crystallinity (thermoplastics) is also required. These steps enable materials selection for manufacturing characteristics, with simultaneous meaningful, real-time, process monitoring and control. According to *Sastry* [2], Poor impregnation of composite materials results in unacceptably high void content, resin-rich areas, or other microstructural defects. And in the meantime, poor consolidation of composites results in similarly unacceptable mechanical properties, with the additional loss of control of matrix properties if curing of resins is not well-controlled with accurate models.

In Figure 1 we can observe of an image that describes the whole curing process.

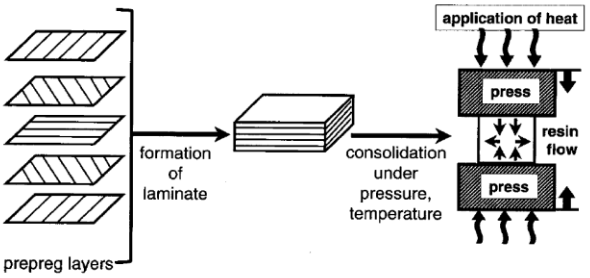

Figure1. Basic processing of a laminated composite, Sastry [2]

The mechanical/rheological behavior of thermosetting polymers during cure is not fully understood. Today's computer simulations of thermoset processing make use of models based on approximations which simply relate the strength properties of thermosets linearly to the degree of cure. However, these assumptions are not valid when modeling thick parts where phase change is temperature and space dependent and significantly contributes to the build-up of residual stresses in the final part.

The cure and consolidation of thermoset composite materials is a complex physical process involving combined heat transfer, resin curing, fiber bed compaction and fluid flow, as mentioned by *Tredoux et al.* [3].

Using a finite difference simulations for either the heat transfer part of this process or for the resin flow part, *Tredoux et al.* [3], planned on performing these steps: *(i)* set up the finite element form of the Fourier heat conduction equation and the Gutowski/Dave resin flow equation through the Ritz formulation, *(ii)* overviewed the computer implementation of these equations and *(iii)* presented selected output results to demonstrate the engineering value of the simulation program.

A similar procedure was implemented by *Blest et al.* [4]. In their paper, they dealt with the modeling and simulation of resin flow, heat transfer and the curing of multilayer thermoset composite laminates during processing in an autoclave. They also took under consideration the Darcy's Law and Stokes' slow-flow equations for the flow model and, for approximately isothermal flows, they developed a similarity solution.

On the other hand, even finding an optimal autoclave temperature and pressure histories for curing of thermoset-matrix composite laminates had been of importance. In order to do so, *Min Li et al.* [1] used a finite element simulation of the heat transfer, curing reaction, and consolidation in the laminate.

We even can find more general procedures in the papers, for example a three-dimensional thermo-kinetic simulation of the liquid composite molding process by *Cheung et al.* [5] was performed. They presented the Galerkin finite element method.

In this paper the control volume method is applied using the general coordinates numerical simulation to model the cure process.

Heat Diffusion Governing Equations

The equation governing the heat transfer process is well established. As described by *Tredoux et al.* [3], for the two-dimensional case, and with the coordinate axes aligned with the principal material axes, this equation has the form:

$$\frac{\partial}{\partial x}\left(k_x\frac{\partial T}{\partial x}\right)+\frac{\partial}{\partial z}\left(k_z\frac{\partial T}{\partial z}\right)+\rho H_R\frac{d\alpha}{dt}=\rho c\frac{\partial T}{\partial t} \qquad (1)$$

And will be recognized as Fourier's heat conduction equation for two-dimensional, transient, orthotropic heat transfer with internal heat generation due to the exothermic curing reaction.

In this equation, T denotes the absolute temperature and K_x and K_z are the respective orthotropic heat transfer coefficients for the composite. H_R is the heat of reaction (J kg $^{-1}$) and $d\alpha/dt$ represents the cure rate (s^{-1}). The degree of cure α varies from 0 (uncured) to 1 (fully cured).

Cure Kinetics

It is said that the exothermic rate of the degree of cure equation for a thermoset resin can be obtained from literature [4]. One of the ways to determine the rate of cure which is used in the formulation is as follows:

$$\frac{\partial\alpha}{\partial t}=A\exp\left(\frac{-\Delta E}{RT}\right)\alpha^m\left(1-\alpha\right)^n \qquad (2)$$

Where A is specified pre-exponential factor, ΔE is the known activation energies, R is the universal gas constant and T represents the temperature in the resin or fibre layer, accordingly. And at the end the parameters m and n are rate constants.

And it is good to know that the degree of cure is temperature dependent, so it is consequently spatially dependent.

Numerical Solution

With substituting the cure rate formulae (2) into the governing equation (1), we started our solution. Using general coordinates within the control volume method, the equation for our solution geometry was discretized. As we know, the cure process is an exothermic phenomenon, and in order to limit the temperatures, a restrictive method in linearization of the source term was implemented.

Numerical Results and Discussion

A numerical two-dimensional cure simulation was conducted for a 15.24×2.54 glass/polyester plate as shown in figure 2.

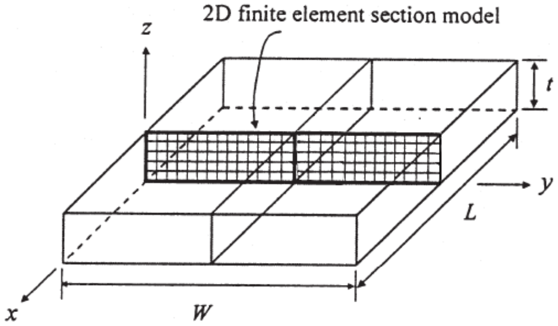

Figure 2. The two-dimensional model of composite

As a glass/polyester material, the Hercules 3501-6 was used and its thermal and kinetic properties can be seen in tables 1 and 2.

Table 1. Material properties of glass/polyester

Density (ρ)	1890 Kg/m3
Polymer specific heat (*Cp*)	1260 J/kg K
Thermal conductivity (K_{zz})	0.2163 W/m K
K_{xx}=K_{zz}	2

Table 2. Cure kinetics for glass/polyester

A (min^{-1})	3.7×10^{22}
E (*J/mole*)	1.674×10^{5}
m	0.524
n	1.476
R (*J/mol K*)	8.31434
H_r (*J/kg*)	77,500

This model was undergone a specific boudary condition temperature as shown in figure 3. As can be seen, at first we have a dramatical increase from room temperature and then this increment is stopped and the material is kept under a constant temperature. After that, the increase in temperature is resumed, and in the end we reach our ultimate goal of cure process, which is a fully cured material. This temperature cycle was applied to every boundary margin of our model. At last, having the results of temperature and degree of cure for our model, we can evaluate our progress. Inorder to do that, the centerpoint node of the domain is selected. In figure 4 the numerical results of our control volume model and the ones of an experimental procedure conducted by *Bogetti et al.* [6] are compared.

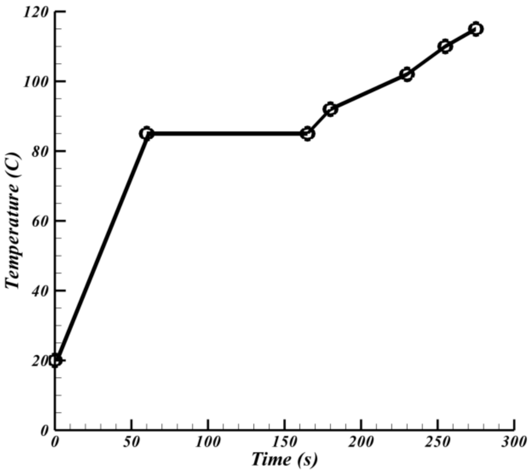

Figure 3. The boundary condition temperature

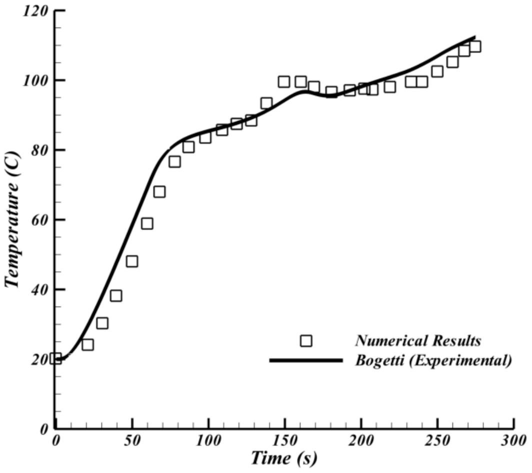

Figure 4. the temperature profile for center-point node compared with experimental results

As we can see, there is a good agreement between our numerical and the experimental results.

Hereby we present a series of results detailing temporal and spatial variation of Temperature and degree of cure within the part. Two time intervals is selected and presented in figures 5 and 6, which are at 70 min into the cure cycle and 250 min respectively.

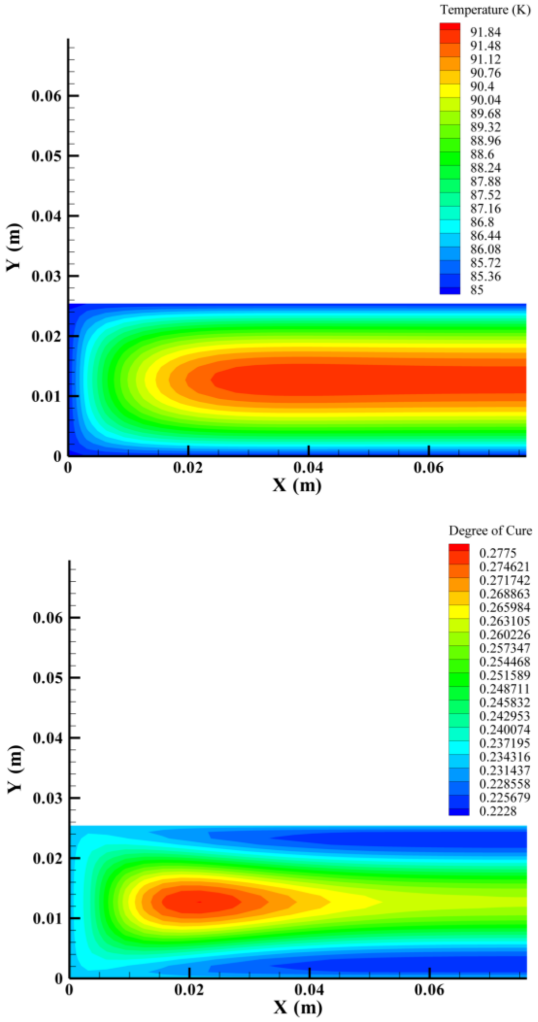

Figure 5. The temperature and degree of cure profiles for center-point node at min 140

The temperature and cure cyle contours for the left side of the model are shown in figures 5 and 6.

In figure 5 we can see that the cure process due to high temperatures in the walls is starting from the left side of the center part and the model is beeing cured along the center portion.

As of figure 6, we can observe the effect of cure process on temperature contours; the increase in temperature causes the cure process to advance, and on the other hand, the exothermic nature of the cure process makes the model hotter which is fully percepted in figure 6. The center part of the model is getting hotter and in return the cure process is being completed in this portion.

As can be seen in these figures, the temperature increases from 85 to 97 and the degree of cure rises from 0.22 to 0.85, and we can observe a difference of 12 degrees in temperature in 50 minutes. It's also visible that we have almost reached the full cure for the center part.

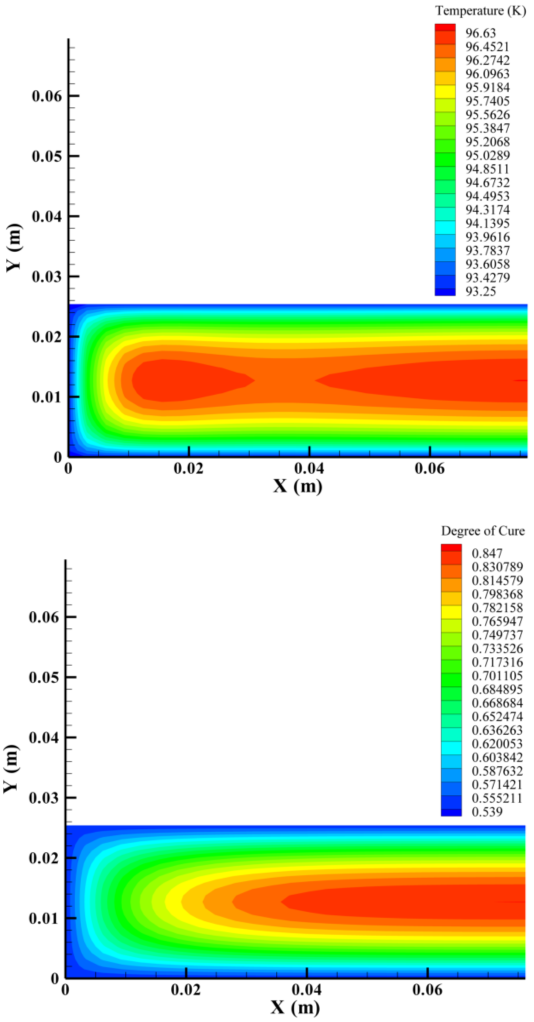

Figure 6. The temperature and degree of cure profiles for center-point node at min 190

Conclusion

In the present work, the control volume method is applied using the general coordinates numerical simulation. Numerical examples are presented depicting the spatial and temporal gradients of temperature and degree of cure within the part. It's also proved that the results obtained from our numerical simulation agrees well with the experimental results found in the literature.

Due to the exothermic reaction of the cure process, there might be an overshoot in temperature, when the cells are about to be fully cured. Inorder to neutralize this effect, a warily method is used to limit the temperatures to a logical threshold.

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