NUMERICAL SIMULATION OF FLOW PHENOMENA IN COMPOSITE MANUFACTURING PROCESSES

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SUMMARY: This paper presents the development and application of a set of numerical procedures for the simulation of the flow phenomena involved in composite manufacturing processes. The procedures developed are based on a general-purpose finite element package. This not only reduces the software development time and cost but also allows the users direct access to all the features pertaining to the FE package. A number of two and three dimensional simulation examples in pre-heating of tools, liquid composite molding and pultrusion are given to demonstrate the capacity and accuracy of the procedures.

KEYWORDS: numerical modeling, cure, heat transfer, flow, pultrusion.

INTRODUCTION

Heat transfer (energy flow) and resin flow through the fibrous reinforcement are two of the most important physical phenomena involved in the manufacturing of advanced composites. A good composite product can only be obtained when the resin is fully impregnated into the reinforcement and properly cured. Temperature distribution, resulting from heat transfer, not only has direct impact on the curing cycle but also significantly affects the mechanical behavior of the tool and the viscosity of the resin. For the manufacturing of a given composite product, proper temperature profile and resin flow pattern must be maintained through tooling design and process control to ensure the quality of the product. Therefore, it is very desirable for tool designers and process engineers to have the capacity to simulate these flow phenomena during the tooling and process design stage. To do this, one usually needs to solve a set of coupled partial differential equations governing the conservation of energy, resin conversion and resin mass. Material properties required for the analysis are usually functions of temperature and the degree of cure which are unknown variables sought by the solution. In addition, the geometry of products and tooling can be complex. Therefore, a closed theoretical solution is usually not possible. A numerical method, such as the finite element method, has to be employed.

In the past two decades, numerous research efforts have been devoted to numerical simulation of composite manufacturing processes. In the context of flow, the problems attempted include heat transfer and cure analysis of the pre-preg process [1-7], heat transfer, resin flow and cure modeling of pultrusion [8-14], and iso-thermal and non-isothermal flow simulation of liquid

composite molding [15-21]. Nevertheless, the present author believes that further development is required for wider application of the simulation in industry. One of the main reasons for this is that due to the general complexity of the problems, most of the simulations reported to date were conducted on specially developed numerical softwares which are normally not available on the market. On the other hand, many companies, particularly those in the aerospace industry, have access to general-purpose finite element packages to perform structural and thermal analyses of composite structures. Therefore, the use of the same packages to model the flow phenomena would be more cost-effective for these companies.

This paper presents the development of a set of numerical procedures for the simulation of composite manufacturing processes at the Cooperative Research Centre for Advanced Composite Structures (CRC-ACS), Australia. The present work differs from most of those reported by other researchers in that all the procedures developed are based on a commercial general-purpose finite element package. The FE package is used to solve the energy and the pressure equations. User programs are developed and interfaced with the package to evaluate the resin cure reaction and/or to advance the flow front. This approach results in not only considerable savings in development time and costs but also makes available to the users all the modeling features of the FE package. Perhaps more importantly, the approach represents a significant step towards computer-integrated-engineering in that it would be more convenient if a structural analysis is to be conducted for the composite part by the same FE package or if the stress is to be coupled into the flow simulation.

THEROTICAL MODEL

Energy equation

Governing the heat transfer process in a composite material is the following energy equation:

$$\begin{aligned}&\overline{\rho c}_p \frac{\partial T}{\partial t} + V_r \rho_r c_{pr}\left(u_x \frac{\partial T}{\partial x} + u_y \frac{\partial T}{\partial y} + u_z \frac{\partial T}{\partial z}\right) = \\ &+ \frac{\partial}{\partial x}\left(\overline{\kappa}_x \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\overline{\kappa}_y \frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(\overline{\kappa}_z \frac{\partial T}{\partial z}\right) + V_r \rho_r H_r R_r\end{aligned} \tag{1}$$

where,
V_r: resin volume fraction;
u_x, u_y, u_z: components of resin flow velocity;
$\overline{\rho}$, $\overline{c}_p$, κ_x, κ_y, κ_z: lumped density, specific heat and conductivity respectively;
H_r: heat of resin reaction;
R_r: rate of resin reaction.
The lumped thermal properties can be evaluated from the properties of the constituents (fibre and resin) by the following equation:

$$\begin{aligned}&\overline{\rho} = V_r \rho_r + (1 - V_r)\rho_f \\ &\overline{c}_p = \frac{V_r \rho_r c_{pr} + (1 - V_r)\rho_f c_{pf}}{\overline{\rho}} \\ &\overline{\kappa}_i = \frac{\kappa_{fi}\kappa_r \overline{\rho}}{(1 - V_r)\rho_f \kappa_r + V_r \rho_r \kappa_{fi}} \quad i = x, y, z\end{aligned} \tag{2}$$

In Eqns. 1 and 2, subscripts *r* and *f* stand for resin and fibre respectively.
The first term on the right hand side of Eqn. 1 represents the energy flow caused by the resin flow and/or the movement of the composite part (convection term). The third term is the internal power generation caused by the resin cure reaction (exothermic term).

The energy equation may be simplified for the pre-preg and pultrusion processes. For a pre-preg material, the resin flow during the curing stage is considered to be insignificant. Eqn.1 can be reduced to:

$$\overline{\rho c}_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(\overline{\kappa}_x \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\overline{\kappa}_y \frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(\overline{\kappa}_z \frac{\partial T}{\partial z}\right) + V_r \rho_r H_r R_r \tag{3}$$

In pultrusion, the fibre is fully impregnated by the resin before entering the die. There is little resin flow except in a small region close to the die entrance. The pultruded part moves in the pull direction at a constant pull speed *u*. Therefore, the energy equation can be rewritten as:

$$\overline{\rho c}_p \left(\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x}\right) = \frac{\partial}{\partial x}\left(\overline{\kappa}_x \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\overline{\kappa}_y \frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(\overline{\kappa}_z \frac{\partial T}{\partial z}\right) + V_r \rho_r H_r R_r \tag{4}$$

Species equation

Similar to the energy, the concentration of the resin species at any material point has to be conserved. This is described by the following species equation:

$$\frac{\partial \alpha}{\partial t} + u_x \frac{\partial \alpha}{\partial x} + u_y \frac{\partial \alpha}{\partial y} + u_z \frac{\partial \alpha}{\partial z} = R_r \tag{5}$$

In the equation, α is the degree of cure defined as the ratio of the total amount of heat evolved during the curing up to time t to the total heat of reaction H_r during the entire curing process per unit mass, i.e.

$$\alpha = \frac{H(t)}{H_{tr}} \tag{6}$$

For the pre-preg process and pultrusion, Eqn. 5 may be reduced to:

$$\frac{d\alpha}{dt} = R_r \tag{7}$$

and

$$\frac{\partial \alpha}{\partial t} + u \frac{\partial \alpha}{\partial x} = R_r \tag{8}$$

respectively.

Darcy's law and pressure equation

On the macroscopic scale, it is a common practice to describe the resin flow through the fibrous reinforcement by the following Darcy's law:

$$\boldsymbol{u} = -\frac{1}{\mu}\boldsymbol{K}\nabla\boldsymbol{P} \tag{9}$$

In the above equation, μ is the viscosity of the resin, $\boldsymbol{u}$ the flow velocity vector:

$$\boldsymbol{u} = \begin{pmatrix} u_x & u_y & u_z \end{pmatrix}^T \tag{10}$$

$\nabla\boldsymbol{P}$ the pressure gradient vector:

$$\nabla\boldsymbol{P} = \begin{pmatrix} \frac{\partial P}{\partial x} & \frac{\partial P}{\partial y} & \frac{\partial P}{\partial z} \end{pmatrix}^T \tag{11}$$

and $\boldsymbol{K}$ the permeability tensor (in principal axes):

$$\boldsymbol{K} = \begin{bmatrix} K_x & 0 & 0 \\ 0 & K_y & 0 \\ 0 & 0 & K_z \end{bmatrix} \tag{12}$$

Applying the condition of incompressibility to Eqn. 9, one obtains the following pressure equation:

$$\frac{\partial}{\partial x}\left(\frac{K_x}{\mu}\frac{\partial P}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{K_y}{\mu}\frac{\partial P}{\partial y}\right) + \frac{\partial}{\partial z}\left(\frac{K_z}{\mu}\frac{\partial P}{\partial z}\right) = 0 \tag{13}$$

It is worth noticing that the above quasi-harmonic equation also governs a number of steady state field problems, including steady state conduction heat transfer.

NUMERICAL IMPLEMENTATION

Numerical procedures are developed to solve the above governing equations approximately for different manufacturing processes. In the procedures, the transient process of heat transfer, resin reaction and resin flow are modeled as quasi-steady by a number of time steps. For page limitation, the solution algorithms used in each time step are described briefly. Refs. 7, 14 and 21 can be consulted for more details.

Solution of temperature

A mixed time integration scheme is used to decouple the convection and the exothermic terms from the rest the energy equation. The energy equation is thus reduced to conduction only and can easily be solved by a FE package.

Nodal control volumes are constructed based on the finite element mesh in such a way that the centers of the control volumes coincide with the nodal points of the mesh. In a time step, the effects of the convection term and the exothermic term are first evaluated from the known temperatures of the previous time step for each of the control volumes. These are then applied as part of the initial/boundary conditions for the solution of the reduced energy equation by a FE package to obtain temperature for the time step.

Solution of cure

An explicit scheme is used to solve the species equation. The solution is conducted on the control volumes by the user program.

Solution of resin flow

The resin flow at each time step is evaluated using the finite element/control volume (FE/CV) method [17,19]. In the method, the pressure equation is first solved by the Galerkin finite element method which is the field solver usually implemented in a general-purpose finite element package. The flow velocity $\boldsymbol{u}$ can then be determined by using Darcy's law. The flow front is advanced using the flow analysis network (FAN) technique [22] based on the control volumes.

It is well known that the FE/CV method does suffer a number of drawbacks. In particular, the method can not result in mass conserved flow unless some restrictions are met in the finite element discretisation [20,23]. In the present work, a scaling scheme is implemented to force the satisfaction of the mass conservation at each time step. The amount of resin mass flow in and out of each control volume is first calculated from the pressure solution. Each of the fully filled control volumes is then checked for the conservation of mass. The resin mass flow out of a nonconserved control volume is scaled up or down accordingly to force the mass conservation in the volume.

Implementation of the procedures

The numerical procedures described above have been implemented on a number computer platforms, including PC, HP and IBM workstations. A commercial general-purpose finite element package LUSAS is used to solve the reduced energy equation and the pressure equation, and to provide data structure for the control volumes. User programs have been written using FORTRAN77 to conduct the control volume analysis and modify the input date file to the FE package. The switching between the FE package and the FORTRAN programs is controlled automatically by a system command.

NUMERICAL EXAMPLES

Electrical heating of tools

One of the frequently used heating methods in composite manufacturing is the integral-electrical heating. In the method, electrical heaters of different shapes, sizes and wattage are directly implemented on a tool and become an integral part of the tool. Better efficiency is achieved by the integral heating as compared to the non-integral heating, such as the autoclave heating. A scheme has been incorporated into the procedures to simulate the temperature control process for the integral-electrical heating.

A three dimensional finite element model was used to simulate the multi-stage heating of the flat tool shown in Fig.1. The tool was made of aluminum and heated by an electrical wire heater. All the surfaces of the tool were exposed to the air.

The predicted temperature response at point B is compared with the experimental response and the preset heating cycle in Fig. 2. Excellent agreement between them was obtained. The

small oscillation on the predicted response was due to a relatively large time increment (0.5 min.) used in the simulation. It would be reduced if a finer time step was used.

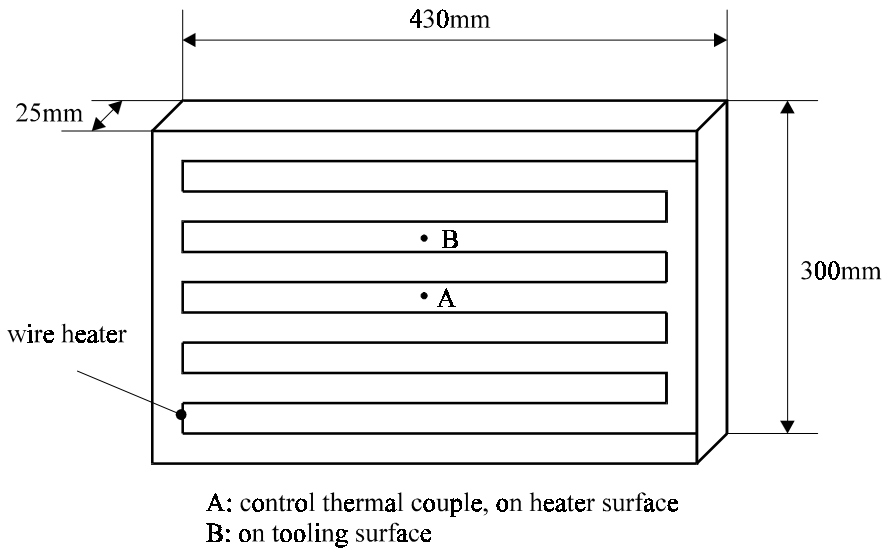

Fig. 1. *Flat tool heated by electrical wire heater.*

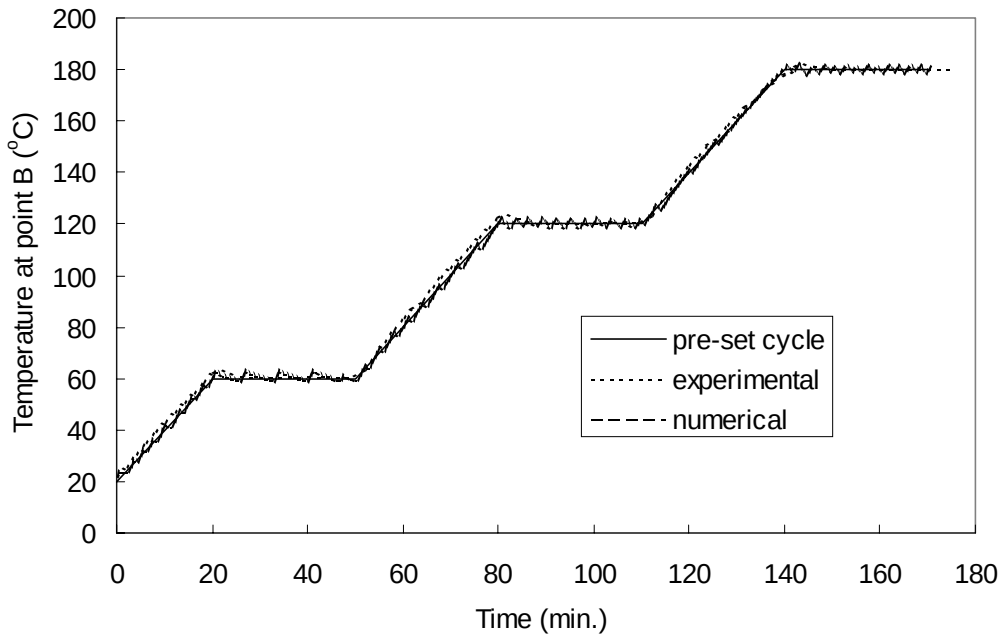

Fig. 2. *Temperature cycle at point B of the flat plate.*

Non-isothermal flow simulation of RFIP

The flow phenomena during the manufacturing of a L shaped composite part by the resin film infusion process was simulated. The tooling assembly for the fabrication is illustrated in Fig. 3. and the tool was heated integrally by the electrical strip heaters. Only a two-dimensional model was used to simulate a cross section of the fabrication assembly

Given in Fig. 4 are the contours of the predicted temperature and viscosity at 98 min., and the degree of cure and the flow front at 141 min. respectively. The predicted total filling time were found to be in good agreement with the experiment.

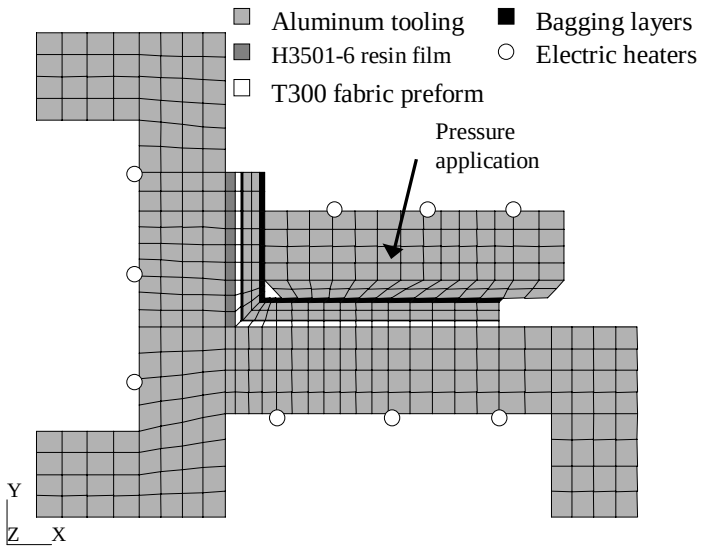

Fig. 3. *FE model for the L section.*

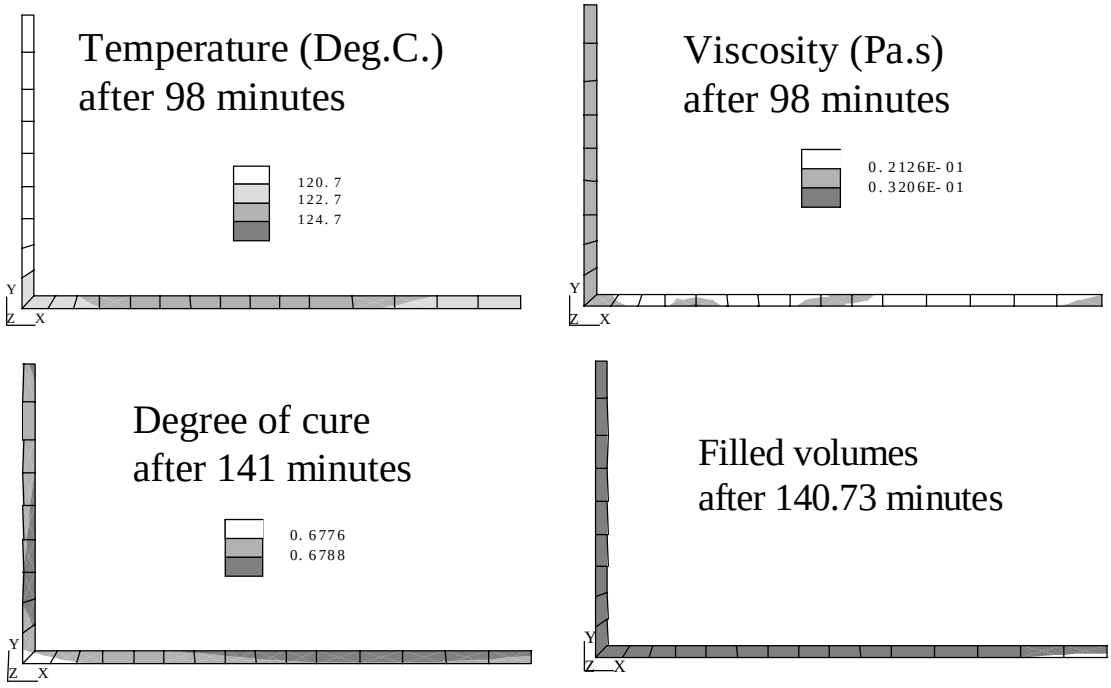

Figure 4. *Contours of the predicted variables for the L section.*

Simulation of pultrusion

One of the pultrusion examples simulated by the present work was the pultrusion of an cylindrical rod. This example was simulated as a steady problem by a number of researchers to validate their numerical models [12,13]. Unlike the previous work, the problem was simulated as a transient one in the present research. The steady state was detected when the changes in temperatures and the degrees of cure obtained for two consecutive time steps were smaller than the given tolerances.

Temperatures and the degrees of cure at the centerline of the rod obtained by the present research are compared with those given in Refs. 12 and 13 in Fig. 6. Both temperature and the degree of cure agreed well with those given in Ref. 12, which were supported by experiments.

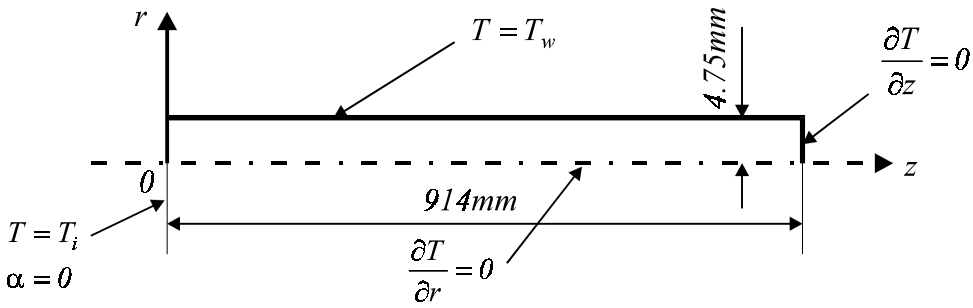

Figure 5: *Schematic of the simulation domain for the rod.*

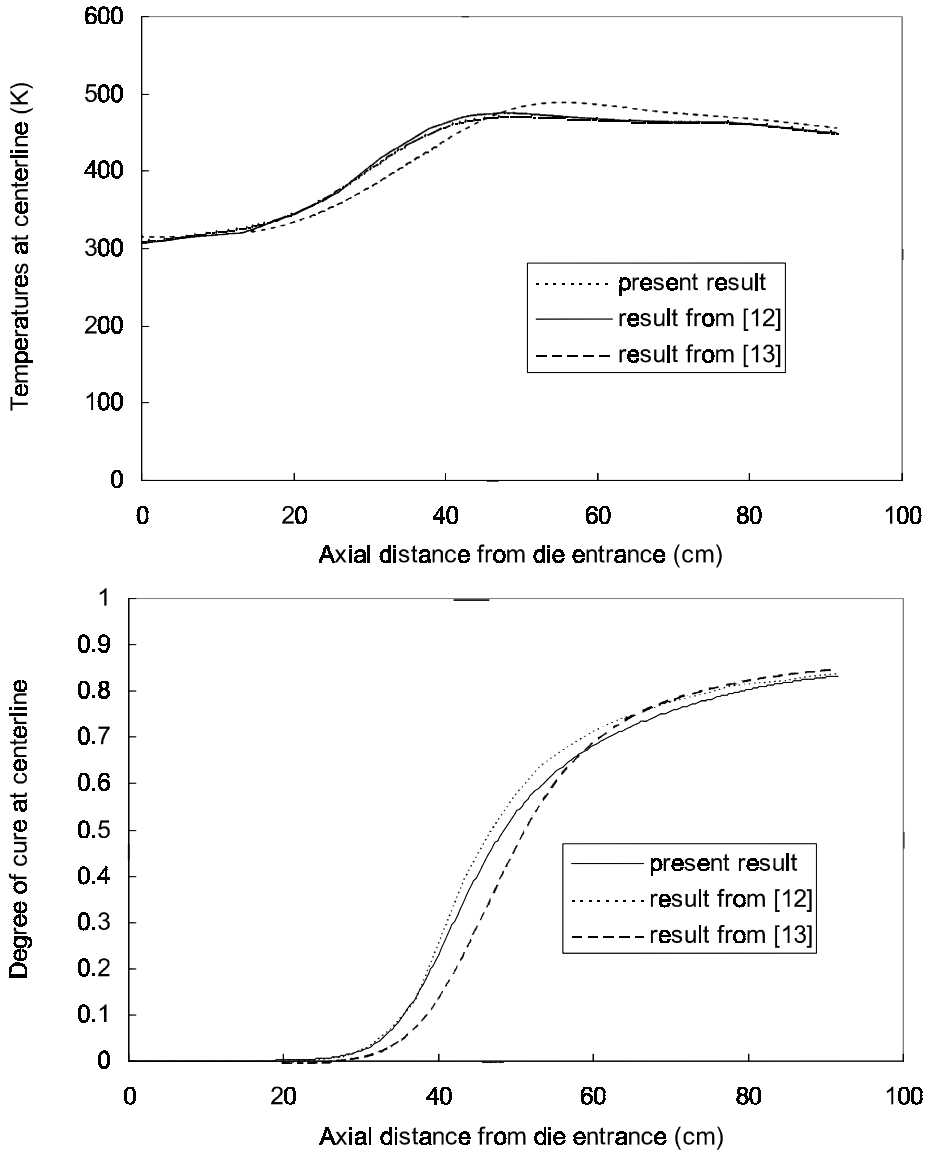

Figure 6. *Predicted temperature and degree of cure at thecenterline of the rod.*

CONCLUSIONS

Numerical procedures have been developed to simulate the flow phenomena during composite manufacturing processes. Comparison of the simulation results with the experimental ones proved that the procedures developed were numerically stable and produced reliable

predictions on temperature, the degree of cure and/or the resin flow pattern. As a result of the present research, the CRC-ACS now has the capacity to simulate the heat transfer, resin curing and flow in the pre-preg processes, liquid composite molding and pultrusion processes in three dimensions.

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