# A TRANSIENT FINITE ELEMENT MODEL FOR PULTRUSION PROCESSING

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## Abstract

Finite element analysis is a general numerical tool for solving the field equations of engineering practice, and this paper demonstrates its use in modeling the nonisothermal cure of pultruded composite material. A very simple grid is used in this case to model a narrow strip of material, and this grid is then solved using a time-stepping algorithm to simulate the passage of the strip along the pultruder die. As time proceeds, heat is conducted into the strip from the heated boundaries at the die walls, and cure proceeds at a rate dependent on the local temperature. The computer model can be used to minimize the time needed for sufficient cure, and helps avoid such processing errors as undercure or thermal degradation.

## I. INTRODUCTION

Although Edisonian innovation will always be important in the development of new materials and processing methods, there is an increasing need for analytical tools which can simulate expensive hardware and laboratory

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experiments. Even when the analytical models must be idealized considerably, they can often serve to sharpen the engineer's intuition of the situation, so that the empirical approach can be more efficient.

This paper demonstrates a simple application of a general finite element code which has been developed to solve the equations governing nonisothermal, reactive, transient viscous flow processes. The code is quite general in its applicability, but this paper will demonstrate that it is also useful in relatively simple situations which might otherwise be attacked by writing special purpose software. We are concerned here with continuous, steady processing operations such as pultrusion or film blowing which have large aspect ratios, the process geometry being much smaller in one dimension than in the others.

Usual finite element grids are awkward in such problems: accuracy generally requires keeping the aspect ratios of individual elements near unity, so having enough elements in the thin dimension to maintain reasonable resolution would require an excessive number of elements in the other. In such problems an alternative approach might be to neglect diffusive transport in the long direction and discretize only a narrow strip of material in the thin direction. This strip could then be followed as it travels along the processing path, so that the long direction is modeled as a time dimension. The two-dimensional code is employed in this case to solve a transient problem in one spatial dimension.

This approach will be outlined using the pultrusion process as an example. The governing equations and their finite element counterpart will be described briefly, and numerical results will be presented for a simulation of an actual pultrusion line for which material and process parameters are known. Finally, we will show the results of some trial situations which are difficult to analyze experimentally.

## II. PULTRUSION PROCESSING

Pultrusion is the name given to a variety of processes for making composite materials consisting of unidirectionally oriented reinforcing fibers in a resin matrix. Price [1] describes several of these processes. Some involve a continuous process where fibers are drawn through a resin bath and then into a heated die to be cured. Other processes involve a partially cured pre-preg composite ribbon which is pulled through a heated die to complete cure. Figure 1 is a schematic representation of a pultrusion process.

As a strip of material enters the heated die region, it experiences a sudden increase in temperature at its outer boundary. Heat is transported into the
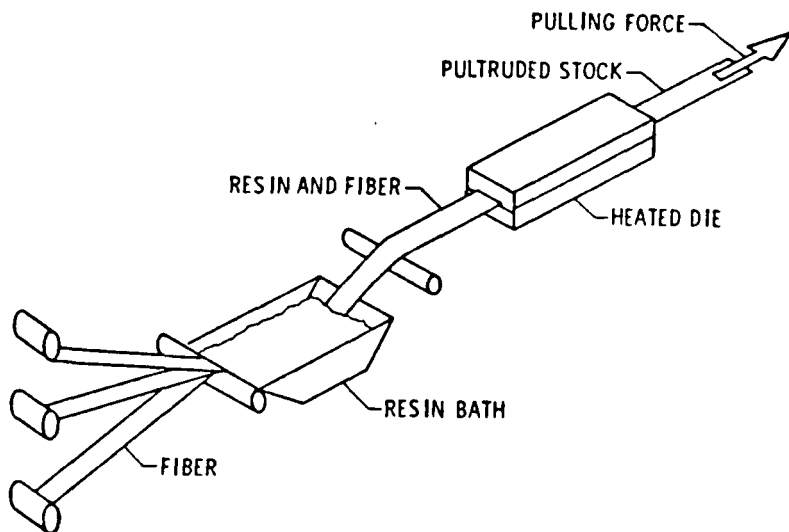
**FIG. 1.** Schematic of pultrusion process (from Price [1]).

material by conduction, which is a relatively slow process in most polymers. As the local temperature increases, so does the rate of chemical reaction. The reaction is exothermic, so an additional heat source will be generated as the reaction proceeds. The problem is then one of coupled, transient heat transfer and chemical reaction.

## III. NUMERICAL MODEL

The equations which govern reactive polymer processing are well known and are available in texts of transport phenomena and polymer processing [2, 3]. They are a set of coupled, nonlinear, second-order partial differential equations which enforce conservation of momentum, energy, and reactive species:

$$\rho[\partial u/\partial t + u \cdot \nabla u] = -\nabla p + \nabla(\eta \nabla u)$$

$$\rho c[\partial T/\partial t + u \cdot \nabla T] = Q + \nabla(k \nabla T)$$

$$[\partial C/\partial t + u \cdot \nabla C] = R + \nabla(k \nabla C)$$

Here $u$, $T$, and $C$ are fluid velocity (a vector), temperature, and concentration of reactive species; these are the principal variables in our formulation. Other parameters are density ($\rho$), pressure ($p$), viscosity ($\eta$), specific heat ($c$), thermal conductivity ($k$), and species diffusivity ($D$). $\nabla$ is the Laplacian operator. The similarity of these equations is evident, and leads to considerable efficiency in the coding of their numerical solution. In all cases the time rate of change of the transported variable ($u$, $T$, or $C$) is balanced by the convective or flow transport terms (e.g., $u \cdot \nabla T$), the diffusive transport (e.g., $\nabla(k \nabla T)$), and a generation term (e.g., $Q$).

$Q$ and $R$ are generation terms for heat and chemical species, respectively, while the pressure gradient $\nabla p$ plays an analogous role for momentum generation. In our polymer problems, the heat generation arises from viscous dissipation and from reaction heating:

$$Q = \tau : \gamma + R(\Delta H)$$

where $\tau$ and $\gamma$ are the deviatoric components of stress and strain rate, $R$ is the rate of chemical reaction, and $\Delta H$ is the heat of reaction. $R$ in turn is given by a kinetic chemical equation; in our model we have implemented an $m$th-order Arrhenius expression:

$$R = k_m \exp(-E/R_g T) C^m$$

where $k_m$ is a preexponential constant, $E$ is an activation energy, and $R_g$ is the gas constant.

These equations are usually not solvable in closed form for problems of practical interest, due partly to the irregular boundary conditions which must be satisfied and also to the nonlinear dependence of material parameters on the solution variables. Recently, however, finite element numerical analysis has grown well beyond its early use as a tool for stress analysis and is now established as a general method for solving the sort of boundary value problems described above.

Several texts [4, 5] demonstrate how the governing equations can be written in an integral form which permits one to satisfy solution criteria over selected subregions ("elements") in the problem domain rather than at every point. The finite element equations can then be obtained by replacing the actual problem variables by interpolations among discrete values at selected nodal points. When this interpolated solution is used in the integral equations, a set of simultaneous algebraic equations can be assembled of the form

$$Ka = f$$

where $a$ is a vector of nodal variables whose values are sought, $f$ is a vector of forces or fluxes, and $K$ is a coefficient matrix relating these quantities. The computer assembles the $K$ and $f$ arrays from the contributions of each element, and then solves for the $a$ vector by Gaussian reduction or other numerical means.

The finite element method can also handle transient problems by using a variety of time-stepping algorithms adapted from the finite-difference technique. The processing problems of interest here involve only the first derivative of time, and for this case the extension to transient problems is simple and inexpensive. When the derivative terms are added, the finite element matrix equations take the form

$$C \frac{da}{dt} + Ka = f$$

where the $C$ matrix stores the inertial influences and $da/dt$ is the derivative vector of the nodal variables. This can be written in finite difference form as

$$C \frac{a_{n+1} - a_n}{\Delta t} + K[(1 - \theta)a_n + \theta a_{n+1}] = f$$

This implicit relation permits the values $a_{n+1}$ at the end of the next time increment $\Delta t$ to be computed from the current values $a_n$. Here the forcing terms $f$ are assumed constant over the time increment, and $\theta$ is a parameter between 0 and 1 which allows the time-stepping scheme to be adjusted between forward and backward differencing. The method is unconditionally stable for $\theta \geq 1/2$, and we have used $\theta = 2/3$ in the simulations to be presented below.

Although many important processing problems have features which strain or exceed the capability of this method—fluid viscoelasticity is a notable example—many other problems can be handled inexpensively and routinely. We have developed a series of element routines for this purpose which operate within the FEAP code written by Taylor and freely available in the Zienkiewicz textbook [4]. Our routines can presently solve the transient momentum, energy, and species equations simultaneously, for Newtonian fluids at low Reynolds' numbers and in domains having fixed boundaries. More detailed descriptions of the formulation are available in earlier publications [6-8].

Our numerical modeling of the pultrusion process avoids the use of flow velocity as an explicit problem variable. Instead, a Lagrangian view is used in which a single strip of material is followed in a time-stepping manner after entry into the heated die (Fig. 2). The progress through this region is then considered only in terms of the heating and reaction effects. Rather than model material flow in an Eulerian laboratory frame, which would require an unwieldy element mesh in two dimensions, the process is idealized as a transient problem in one spatial dimension. The simple 13-element grid of Fig. 2, refined at the outer edge to capture the boundary effects more accurately, was used for all of the simulations to be discussed below.

This approach to the pultrusion analysis differs from the usual scheme of first reducing the general governing equations to fit the problem at hand—in this case a one-dimensional transient formulation. Instead, the code is written to solve the general equations as outlined earlier, and only the form of the input dataset changes to effect the particular solution desired. This method may seem unconventional to the reader accustomed to seeing a development of specific equations for particular cases which are then attacked by closed-form or numerical means, but it is arguably more general and economical.
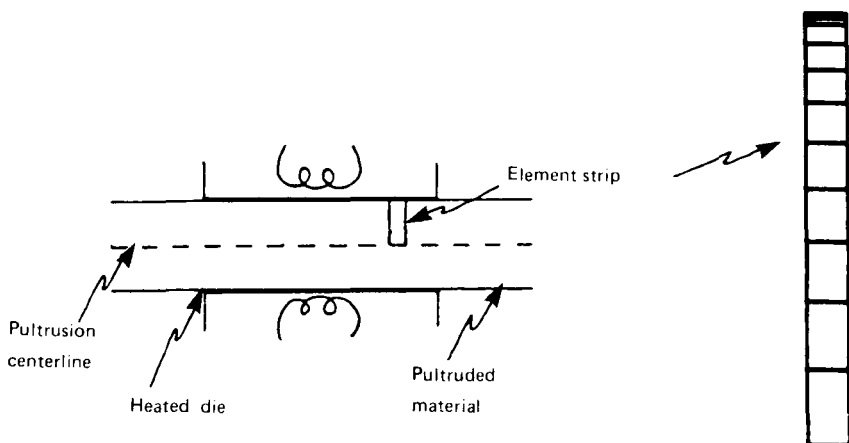


FIG. 2. Pultrusion heater die and element mesh.

## IV. MODEL RESULTS AND DISCUSSION

### A. Simple Conduction

As an initial check of the computer model, a simple reactionless conduction problem for which a closed-form solution is available was modeled using a strip of elements initially at constant temperature $T_1$. One edge is constrained at this temperature, while the other is suddenly exposed to a higher temperature $T_2$. Figure 3 shows the theoretical transient temperature profiles along the strip as given by the solution in Schlichting [9] and the computed results obtained using log time stepping at three time steps per decade. At short times a thermal boundary layer develops near the heated edge, and at long times the temperature profile in the strip becomes linear from $T_1$ to $T_2$. Figure 3 also shows the computed temperature profile at one time when only one time step per decade is used; the coarser time steps lead to a reduction of accuracy, as expected.

### B. First-Order Isothermal Reaction

A trial pultrusion run with very high thermal diffusivity (to enforce rapid conduction of heat from the heated edge to the center, and thus essentially
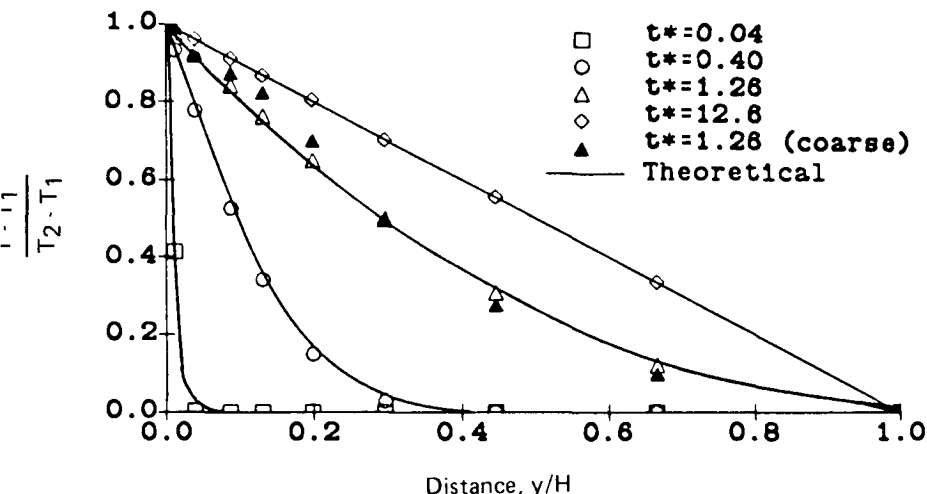


FIG. 3. Theoretical and model transient temperature profiles for a simple conduction problem. Dimensionless time $t^* = 4(\sqrt{at})/h$.
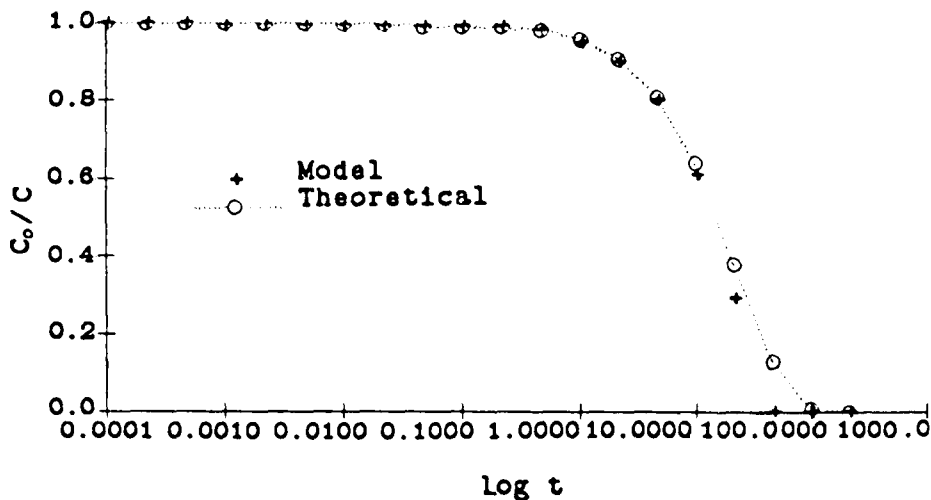
FIG. 4. Theoretical (closed-form solution) and model (computer solution) reactant concentration histories for a first-order isothermal reaction.

uniform and steady temperature profiles throughout the material) was made to verify the reaction modeling capabilities of the code. A first-order reaction was modeled with the initial concentration of reactants set at 1.000, and the results are shown in Fig. 4. The plotted points are the computed reactant concentration values averaged over the length of the strip at each time. Excellent agreement between computed and closed-form values is obtained over most of the reaction history. At longer times some error is observed, probably due to the logarithmically increasing size of the time steps.

## C. Pultrusion Simulations

The width of the pultrusion stock is taken to be substantially greater than the thickness, so that gradients across the width can be neglected. We have modeled the pultrusion of "thin" (2 mm) and "thick" (2 cm) specimens, using the 13-element strip stretching from the pultrusion centerline to the heated edge as shown in Fig. 2. The boundary conditions for both simulations were set to give a constant temperature at the heated edge and zero temperature and concentration gradients at the centerline. The material modeled was a real epoxy–graphite composite whose curing kinetics and pultrusion behavior has been studied by Price [1]; his material and reaction parameters are listed in Table 1.

**TABLE 1**
**Material and Reaction Properties**
**for Graphite–Epoxy Composite**

| Property | Value |
|---|---|
| Thermal conductivity, W/m·°K | 1.0 |
| Density, kg/m³ | 1500.0 |
| Specific heat, J/kg·°K | 1000.0 |
| Reaction heat, J/kg | 60.3 |
| Reaction order | 1.0 |
| Preexponential constant, s⁻¹ | $4.16 \times 10^4$ |
| Activation energy, J/mol | $5.6 \times 10^4$ |

Figures 5 and 6 are the transient temperature and reactant concentration profiles for the 2-mm "thin" pultrusion problem. The temperature profiles become essentially constant at 490 K within 10 s and stay constant throughout the course of the reaction. This result is in reasonable agreement with that of Price [1], who used finite difference methods to show that a uniform temperature profile was reached in about 3 s, after which the temperature in the strip remained essentially constant.

The reaction in this case lags behind the temperature rise, and except at the very beginning of the reaction at the heated edge, the reactant concentration profiles are essentially flat across the thickness of the strip. A noticeable decrease in reactant concentration occurs between 0.1 and 2.2 s, and the reaction is complete between 20 and 40 s after the pultruded strip enters the heated zone.

Figure 5 shows the closed-form predictions for temperature distributions in the simple conduction problem corresponding to the pultrusion boundary conditions, but without reaction, at two times [10]. The computed temperature profiles are at or slightly below these theoretical levels. At this point the reaction has not yet begun, so the close agreement between the theoretical solution and the code results is another confirmation of the model accuracy. At longer times, when the reaction has progressed substantially, the temperature profile still remains flat at about 490 K. Heat from the reaction is small compared to the material's heat capacity, and in this case is able to diffuse out of the thin specimen quickly.

Figures 7 and 8 are the transient temperature and reactant concentration profiles for the 2-cm "thick" pultrusion strip at 490 K. At 100 s the center
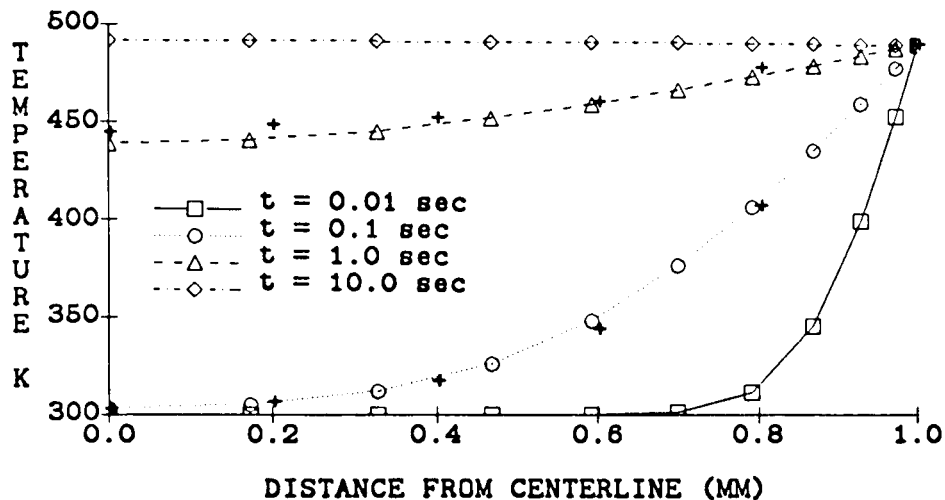
**FIG. 5.** Transient temperature profiles for a 2-mm pultrusion strip cured at 490 K (+ = theoretical temperature profiles with no reaction present).
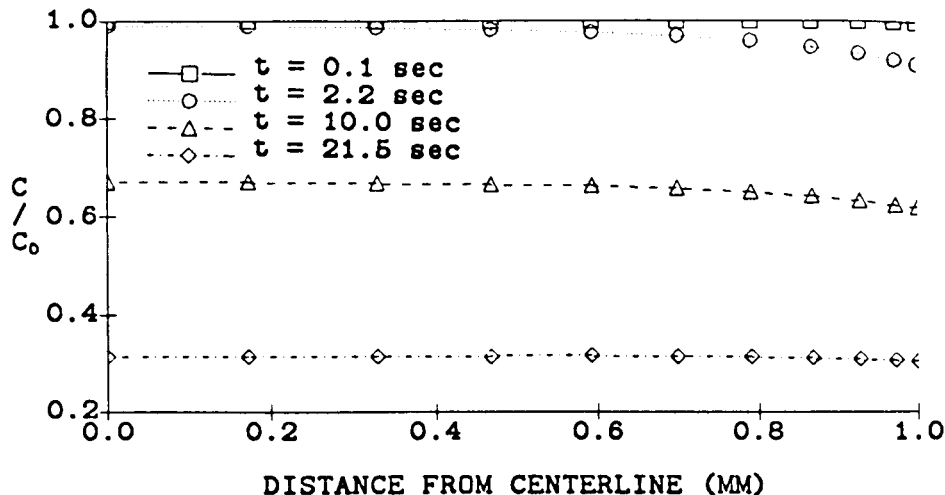


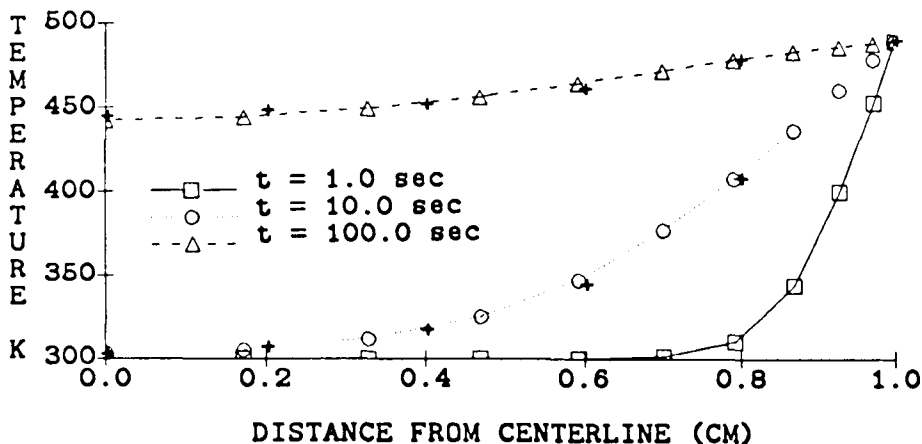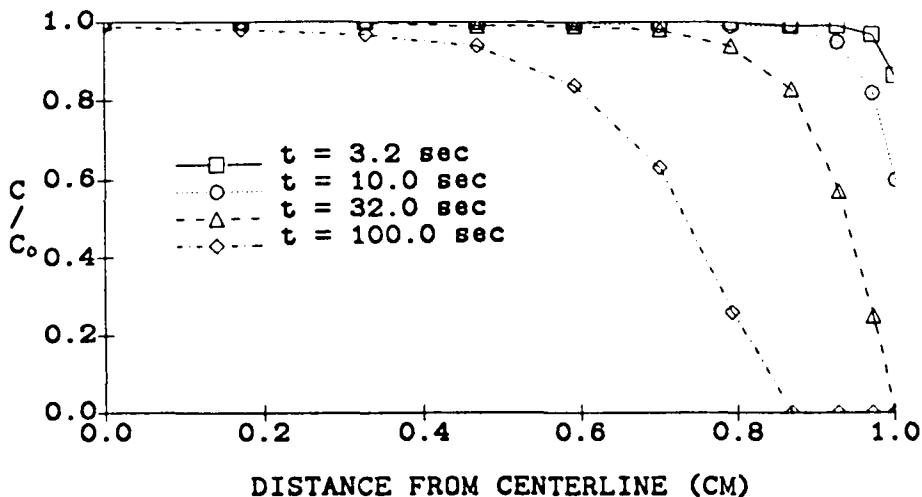**FIG. 6.** Transient concentration profiles for a 2-mm pultrusion strip cured at 490 K.

FIG. 7. Transient temperature profiles for a 2-cm pultrusion strip cured at 490 K (+ = theoretical temperature profiles with no reaction present).



FIG. 8. Transient concentration profiles for a 2-cm pultrusion strip cured at 490 K.

of the strip has still not reached the heater temperature. The edge of the strip has reacted completely at this point, while more than half the thickness of the strip is essentially unreacted. This is clearly an undesirable configuration for any kind of industrial application; the strip would take much too long to cure. Another run was made, this time with the heater temperature increased 25°C to 515 K, to see if this would decrease the curing time for the specimen. Figures 9 and 10 are the temperature and reactant concentration profiles for this test. The 25°C increase in curing temperature provided only a slight increase in the amount of the strip cured after 100 s. Based on this information, it would seem that a 2-cm thick pultrusion of this material is an impractical process if heating is by conduction only. This is an example of how this model could be used as a design tool. By using the model to make preliminary predictions on the feasibility of a process, or on how to optimize a process, the need for expensive process experimentation can be reduced.

It is interesting to simulate a process in which the exothermic reaction heat cannot be removed quickly enough by thermal conduction, leading to
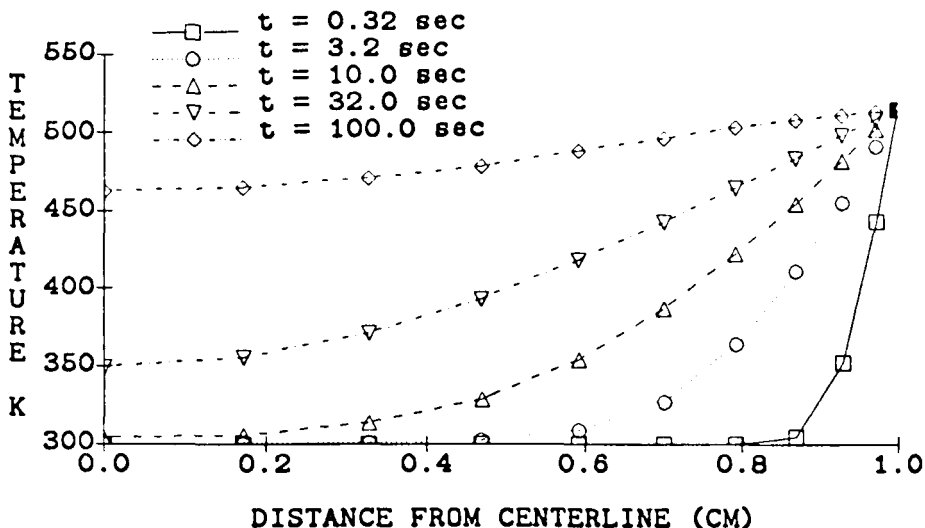


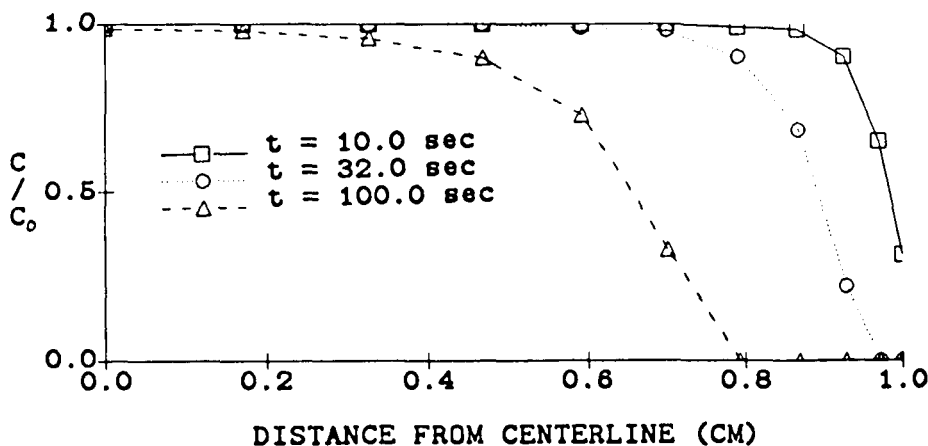FIG. 9.  Transient temperature profiles for a 2-cm pultrusion strip cured at 515 K.

**FIG. 10.** Transient concentration profiles for a 2-cm pultrusion strip cured at 515 K.

catastrophic temperature rises. Clearly, such processes are studied more safely by computer simulation than by laboratory experimentation. To demonstrate this effect, the thermal capacity of the material was artificially set to a low value by adopting a density of a 1 kg/m$^3$. All other material parameters are the same as for the graphite-epoxy composite. Figure 11 shows the dramatic increases in internal temperature for this combination of input parameters. This extreme situation is an example of the complications that can arise when exothermic reactions are present, and the value of theoretical modeling as a means of avoiding catastrophes in the laboratory or production line.

## V. CONCLUSIONS

The pultrusion of the epoxy-graphite composite modeled in this work was seen to be practical for thin (2-mm) ribbons, but the thicker (2-cm) specimen took too long to cure at a given temperature to be practical. The cure of a hypothetical low-density material demonstrated the danger present when an exothermic reaction has a significant heat of reaction compared to the heat capacity or conductivity of the material.

This use of finite elements does not really use the method's powerful ability to treat irregular boundaries, but does serve to illustrate how the
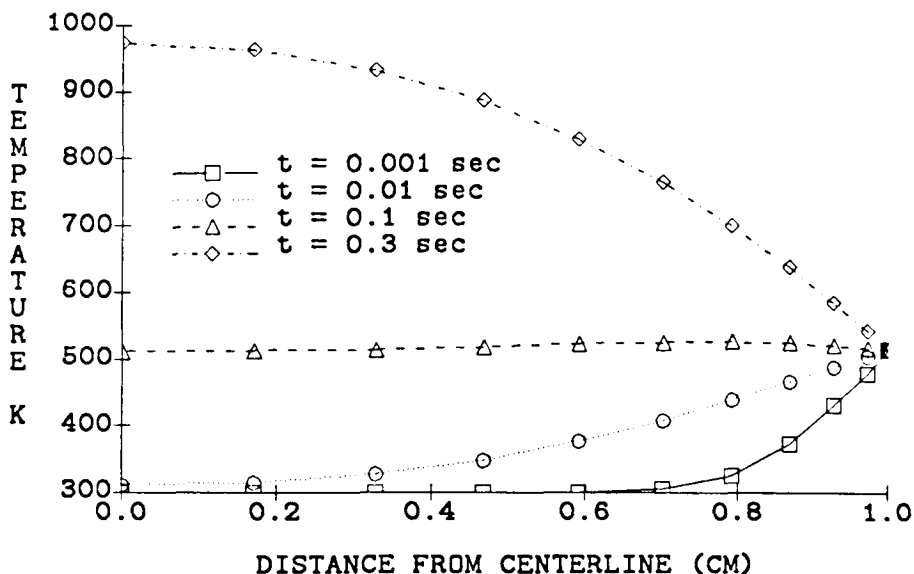
**FIG. 11.** Transient temperature profiles for a hypothetical low-density 2 cm pultrusion strip cured at 515 K.

generality of the technique can be exploited to solve materials problems without resorting to special-purpose software. Although the pultrusion problem can be treated with finite differences [1], such treatments usually involve code development specialized to a particular case; here it was only necessary to construct a suitable input dataset. Even with the higher computational overhead often associated with finite element codes, these problems took less than a second of processor time on a mainframe computer. With some further streamlining, it might be possible to use the code on a dedicated computer for pultrusion control and optimization.

### Acknowledgments

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