Efficient Modelling Techniques for Predicting Processing Residual Stress and Deformation in Composite Parts

Nima Zobeiry, Ali Rasekh, Reza Vaziri[*], Anoush Poursartip

Composites Group, Departments of Civil Engineering
and Metals and Materials Engineering, The University of British Columbia
Vancouver, British Columbia, Canada, V6T 1Z4

ABSTRACT: Motivated by a desire for more efficient process modeling of composite structures, we present two numerical techniques for the optimization of both setup issues and runtimes while still using relatively complex constitutive equations. Firstly, we consider the use of viscoelastic (VE) constitutive equations for modeling the mechanical response of thermoset matrix composites during cure. We show that a cure hardening linear elastic approach is a valid pseudo-viscoelastic (PVE) approximation to the hereditary integral-based viscoelastic solution offered in the literature. PVE formulations are significantly more efficient and easier to implement than VE formulations and there is therefore a great incentive to use them in process modeling. Secondly, we show that the implementation of specially constructed super elements in the thermo-chemical analysis provides similarly useful efficiencies, in this case in setting up the problem and in runtimes.

KEYWORDS: Processing; Process Modelling; Thermoset Matrix; Viscoelasticity; Super Finite Element Modelling; Thermo-Chemical Analysis.

INTRODUCTION

Residual stresses are generated in polymer matrix composites during processing: with thermoset polymer matrices, the main source of these residual stresses are the relative volume changes of the matrix, due to both thermal and chemical effects; however, phenomena such as mechanical interaction with the tooling during cure can also contribute. The magnitudes of the residual stress are dependent on process conditions as well as material properties, geometry, and lay-up of the laminate. Residual stresses are undesirable, as they can lower the strength of the structure and cause geometric distortions.

There are a large number of models in the literature, of varying degrees of complexity and sophistication, which attempt to predict the development of residual stress and consequent deformation of a composite structure. The simplest are analytical methods that provide insight and even quantitative solutions for simple geometries or cure cycles, e.g. [1]. However, for a comprehensive analysis there is need for a numerical solution, nowadays typically a Finite Element Method (FEM) solution. Many researchers use commercial finite element codes, with user defined subroutines where needed; others, such as our group, have developed special purpose FEM codes: in our case COMPRO [2]. Typically, there is a thermo-chemical module, that solves the thermal problem, including the complex applied boundary conditions and the exothermic response of the matrix material as it cures; a flow module that allows for resin flow prior to gelation; and a stress/deformation module that allows for the buildup of stress due to thermal, chemical, and mechanical interactions between the fibre, matrix, layers, and tooling and inserts. COMPRO uses a two-dimensional finite element model to simulate the various phenomena that take place during processing of composite structures. The software has been extensively used to model the process-induced distortions in industrial size composite structural components.

---

[*] Author to whom correspondence should be addressed (email: reza.vaziri@ubc.ca)

A major problem is that for even simple problems, a full three-dimensional, thermo-viscoelastic solution can be very expensive: both in terms of characterizing the materials and accurately defining the initial and boundary conditions and then in terms of computer run-times. There is therefore industrial interest in the tradeoffs between complexity and accuracy.

In this paper, we present two numerical techniques that allow for an optimization of both setup issues and runtimes while still using relatively complex constitutive equations. Firstly, we consider the use of viscoelastic constitutive equations for the mechanical response. We show that a cure hardening linear elastic approach is a valid pseudo-viscoelastic approximation to the hereditary integral-based viscoelastic solution first presented by Kim and White [3]. Secondly, we show that the implementation of higher order elements in the thermo-chemical module provides similarly useful efficiencies, in this case in setting up the problem and in runtimes.

CONSTITUTIVE MODEL

Numerous studies have been undertaken to develop appropriate constitutive models for the development of residual stress during cure. The most sophisticated models have been based on the hereditary integral form of viscoelasticity [3]. Simpler models have also been implemented. Of interest here is the simplified and numerically efficient constitutive model, the so-called cure hardening instantaneously linear elastic (CHILE) formulation within COMPRO, which accounts for the evolution of elastic properties of the polymer with time and temperature during cure, but ignores the viscoelastic relaxation behaviour [2]. This approach has been quite effective in predicting the distortions of many practical, often complex, composite structures employed in the aerospace industry. However, to date the CHILE approach has not been reconciled with the fundamentally more correct viscoelastic approach.

Here we compare the CHILE approach with the computationally intensive viscoelastic approach. It is shown that if an appropriately calculated time or frequency is chosen, at which the elastic modulus of the polymer is evaluated, the CHILE model predictions for the uniaxial loading of a fully constrained block of polymer undergoing a given cure cycle compare very well with those computed using the full viscoelastic model.

Almost all the existing VE models in the literature use the following hereditary integral formulation:

$$s(t) = \int_0^t E\big(x(t) - x'(t)\big)\frac{de}{dt}\,dt \tag{1}$$

where a is the degree of cure and T is the temperature. Also, x and x' are the reduced time variables defined as:

$$x(t) = \int_0^t \frac{1}{a_T(a,T)}\,dt' \;; \quad x'(t) = \int_0^t \frac{1}{a_T(a,T)}\,dt' \tag{2}$$

in which a_T is the shift factor facilitating time-temperature superposition and t' is a dummy time integration variable.

In contrast, with the CHILE approach an elastic modulus, which is a function of temperature and degree of cure, is used. The constitutive model for this case takes the following form:

$$s(t)=\int_0^t E'(a,T)\frac{de}{dt}dt \tag{3}$$

in which E' is the modulus of elasticity as a function of temperature and degree of cure.

The material truly shows viscoelastic behaviour, and thus in experimentally determining E' a definition of modulus is needed. This modulus can be defined as the viscoelastic relaxation modulus evaluated at a certain time or the dynamic viscoelastic storage modulus at a certain frequency. In Reference [7], a mathematical procedure has been used to find out the conditions under which the CHILE model is comparable to a VE formulation. Given some very reasonable assumptions, the VE integral formulations can be simplified to yield the CHILE model. In reality, the CHILE model, when calibrated as described in [7], is a Pseudo-Viscoelastic (PVE) model. It will be shown here that such a PVE model can yield results close to those of a VE model, while being much easier to characterize, implement, and run for practical cases.

The simplification procedure presented in [7] yields a time at which to evaluate the modulus so that it matches the VE modulus. In brief, the form of the modulus response does not matter; the critical variables are the shift factor and the reduced time. This is perhaps not surprising, as inspection of Equations (1) and (3) shows clear similarities between them. The shift factor at the end of a typical cure cycle is exponentially larger than those during the cycle. This is a reflection of the fact that temperature has a large impact on the rate of relaxation of modulus. This causes the first reduced time in Equation (1) become negligible compared to the second one, x'. Therefore, the modulus will be only a function of the dummy time, t, which in turn is only a function of the *current* temperature and degree of cure thus making the VE formulation very similar in form to the PVE formulation. According to this procedure the accuracy of the stresses increases towards the end of the cure cycle. However, the rate of change of the shift factor is so high that the results at other times during the cycle will be accurate as well.

The simplification procedure outlined above results in a *time* at which to evaluate the modulus, but there is a great incentive to use a frequency-based model, since it corresponds to using a dynamic test with the given frequency, a common method in polymer characterization. It will be shown that the values of calculated moduli based on time and frequency correspond to one another and therefore the frequency-based method can also be used to predict the stresses accurately.

We claim only that the PVE/CHILE approximation works for a curing thermoset polymer undergoing reasonably conventional cure cycles. However, it is important to note that the required assumptions cover a wide range of conventional cure cycles and are valid for most practical cure cycles. In the next section, some numerical runs for a one-dimensional case study are used to compare CHILE/PVE and VE models.

Numerical Predictions

A one-dimensional constrained 3501-6 epoxy resin structure undergoing a cure cycle is considered. Both cure shrinkage and thermal strains are included. The advancement of cure is also taken into account using a thermo-chemical model. The parameters are all based on the model in [3]. Here, the material is taken through a two-hold cure cycle, as shown in Figure 1. The stresses generated through the cure cycle are calculated from both models and are presented in Figure 2. The CHILE/PVE results are based on calculating the elastic modulus at a certain time from the relaxation modulus using different values of time.

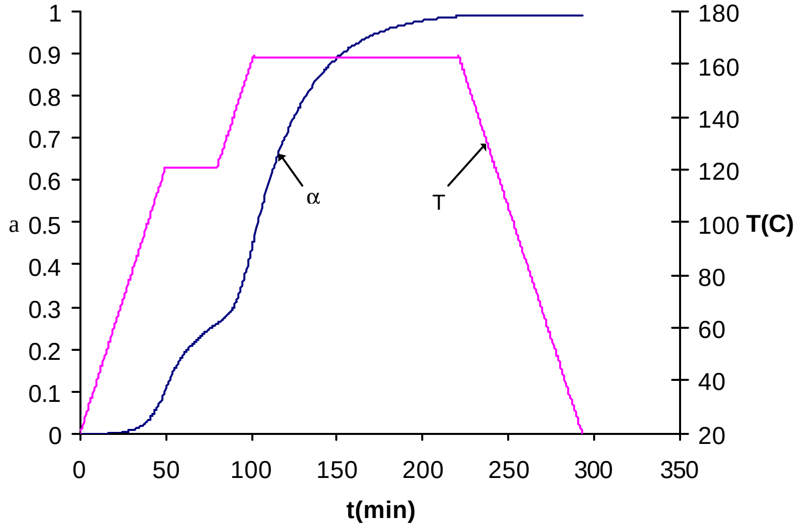

Figure 1 *Profiles of temperature and degree of cure in a two-hold cure cycle for 3501-6 resin.*

Figure 2 shows that the PVE predictions agree very well with the VE predictions for an evaluation time of 3 minutes. The simplification procedure indicates that in this case a time of 3.07 min should have been used. As can be seen, not only is the PVE prediction for an evaluation time of 3 min very good, but also the predictions are not overly sensitive to the value.

It was mentioned that the time- and frequency-based formulations closely correlate. An approximate relation between the moduli evaluated using the two methods is given in Reference [4] as follows:

$$E(t) = E'\left(w = \frac{1}{t}\right) \tag{4}$$

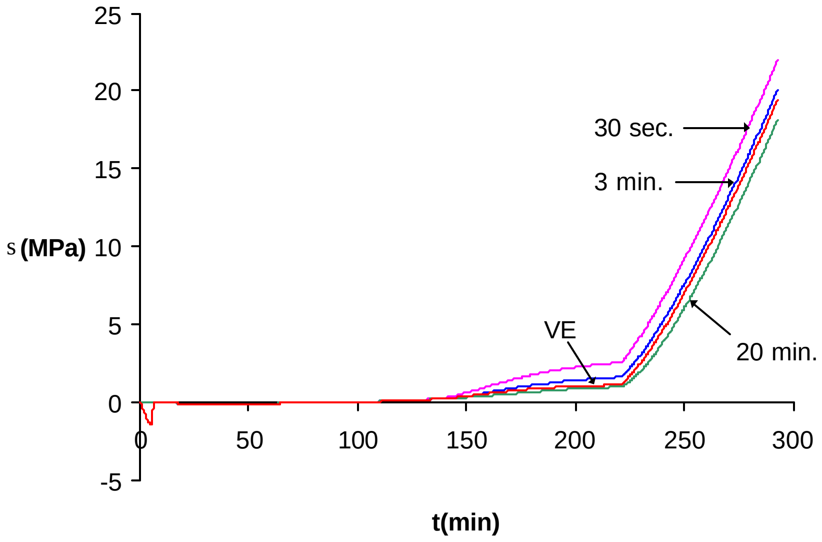

Figure 2 *Comparison of stress profiles for constant time Pseudo- and Viscoelastic models in a two-hold cure cycle, 3501-6 resin.*

An example is given here to show the validity of this correlation. Figure 3 presents residual stresses predicted as resulting from a conventional one-hold cure cycle, calculated using both times and frequencies. There is a strong correlation between the two sets of moduli, based on the previous equation. As a result, therefore, one can confidently choose an appropriate frequency prior to running the numerical code.

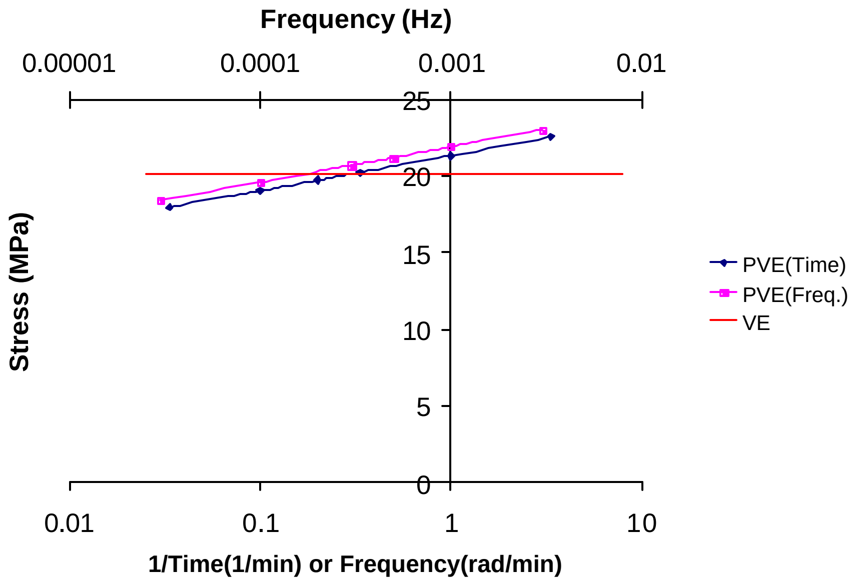

Figure 3 *Correlation of time- and frequency-based PVE models based on residual stresses, one-hold cycle with* T_{hold} *= 180 °C, 3501-6 resin.*

EFFICIENT DISCRETIZATION METHOD

In order to model process-induced deformations and stresses in complex three-dimensional structures it is necessary to have efficient computational techniques that do not require the full discretization of the domain of the problem consisting of both the composite material and the process tool (mould). This will not only lead to a dramatic reduction in computational times but also in data preparation and mesh generation [5][6]. In the absence of such techniques, the composite structure will have to be modelled in all three dimensions using brick elements leading to a huge computational effort both in mesh generation and solution of equations.

Thermo-chemical analysis is an important step in the process modelling of thermoset polymer composites as it deals with the quantification of the spatial and temporal distribution of the temperature and the polymer degree of cure. Both these variables are responsible for the material property development of the composite during processing and in turn drive the residual stresses and deformations that will be generated.

To this end, a super finite element technique is presented here to provide an accurate and efficient prediction of the temperature field at any time during the process cycle. The basic idea is to develop an element that is capable of solving a 3D heat transfer problem in plate structures using an analytical series approximation in the through thickness direction and a regular FE model in the plane of the plate. It can be shown [8] that unless radical changes occur in the boundary conditions and/or excessive internal heat is generated within the solid, the first few terms in the analytical series are sufficient to calculate the through thickness distribution of temperature in the plate.

There follows a brief outline of the super element formulation, and corresponding results are presented for the 2D thermo-chemical analysis of a composite part in order to facilitate comparison of its accuracy and efficiency with the full-blown finite element code, COMPRO. Similar concepts can be used to mathematically construct a three-dimensional super element.

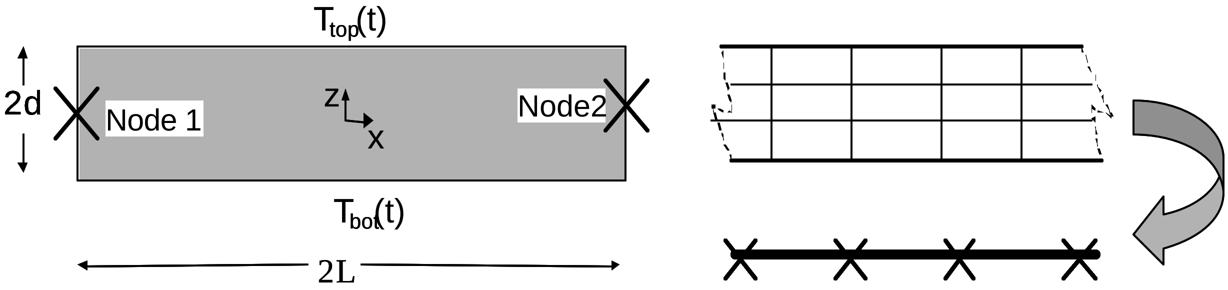

Figure 4 *Typical element used in our analysis (left) and the reduction of discretization in the FEM mesh with the use of super elements (right)*

Governing Equations

The governing equations for the thermo-chemical analysis of a 2-D orthotropic body as shown in Figure 4 consist of a partial differential equation (PDE) for heat transfer coupled with a cure kinetics equation that describes the evolution of the degree of cure as follows:

$$\begin{aligned} & rC_v \frac{\partial T}{\partial t} = k_x \frac{\partial^2 T}{\partial x^2} + k_z \frac{\partial^2 T}{\partial z^2} + H(x,z,t) \\ & H(x,z,t) = rH_R \frac{\partial a}{\partial t} \\ & \frac{\partial a}{\partial t} = g(T,a) \end{aligned} \tag{5}$$

In the above, T denotes the temperature, r is the density, C_V is the specific heat, k_X, k_Z are the components of thermal conductivity in the x and z directions, respectively, H_R is the heat of reaction and a is the degree of cure.

In the proposed super element formulation, the temperature field is approximated in the following series form:

$$T = a(x,t)z + b(x,t) + \sum_{n=1}^{\infty} W_n(x,t) Z_n(z) \tag{6}$$

where Z is a trigonometric shape function which is selected based on the operative homogeneous boundary conditions (B.C.'s) at the top and bottom of the composite part; W is approximated using the conventional finite element method; and a and b are dependent on the non-homogeneous B.C.'s.

Using the Galerkin based weak formulation and FE discretization, we obtain the following system of algebraic equations for the unknown nodal variables W_i (or $\boldsymbol{W}$ in vector form):

$$r\, C_v \boldsymbol{N}\dot{\boldsymbol{W}} + \left[\left(k_x / L^2\right)\boldsymbol{N}^P + \left(b_i k_z / d\right)^2 \boldsymbol{N}\right]\boldsymbol{W} + \boldsymbol{Q}(t) = 0 \qquad (7)$$

where $\boldsymbol{N}$ and $\boldsymbol{N}^P$ are matrices that are calculated from the integration of the in-plane shape functions and spatial derivative of the element shape functions, respectively; b_i is the i^{th} eigenvalue of the PDE and is dependent on the B.C., and $\boldsymbol{Q}$ is obtained from the weighted integral of the internal heat generation term. The time integration in the above equation is carried out using a backward Euler finite difference scheme.

Numerical Verification Example

In order to verify the above technique we consider the case of a 60 mm-thick cross-ply carbon fibre-reinforced AS4/8552 composite material undergoing the two-hold autoclave temperature cycle shown in **Figure 5**. The problem is analysed using both the conventional finite element method (COMPRO) and the current super element method. We consider the case where the temperature at the top and bottom surfaces of the composite are specified to be distributed uniformly and follow the time histories shown in **Figure 5**. It should be noted that these temperature profiles, which are used here as input to the super element model, are obtained from the numerical heat transfer analysis (using COMPRO) of the combined composite material and the tool subjected to the convective thermal boundary conditions (autoclave temperature profile) imposed on all exterior surfaces.

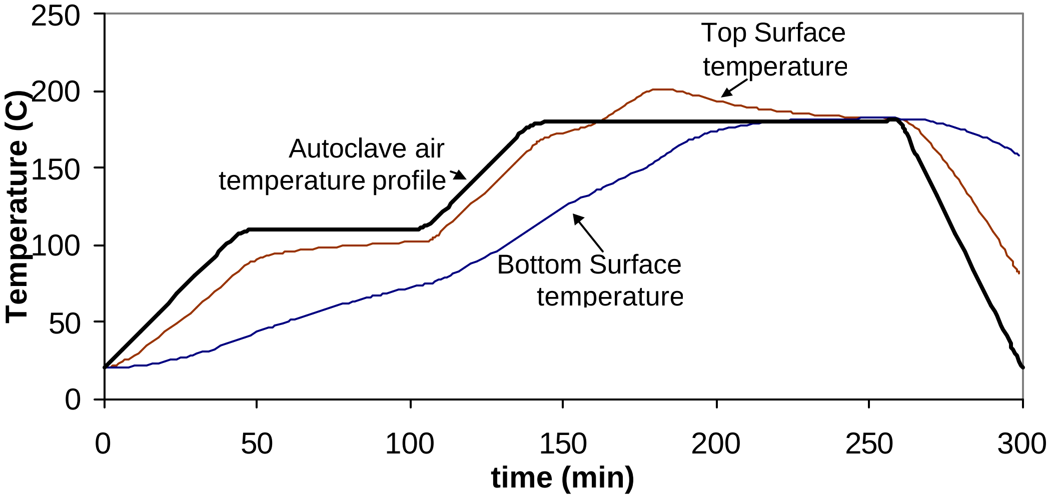

Figure 5 *The autoclave temperature cycle as well as the temperature profiles applied to the top and bottom surfaces of the composite material used for the numerical verification example.*

In this study the cure kinetics model is identical to that used in [2] and the relevant material properties are as follows:

$$r = 1.581\ \mathrm{kg/m^3} \qquad C_v = 9.39 \times 10^2\ \mathrm{J/kgK}$$
$$k_x = 3.74\ \mathrm{W/mK} \qquad k_z = 0.4334\ \mathrm{W/mK}$$
$$H_R = 5.40 \times 10^5\ \mathrm{J/kg} \qquad V_f = 0.427\ \text{(fibre volume fraction)}$$

Appropriate transverse shape functions are selected to satisfy the essential boundary conditions on the upper and lower surfaces of the composite:

$$Z_i(z) = \begin{cases} cos\left(i\dfrac{p}{2}\dfrac{z}{d}\right) & i = 2k-1 \\ sin\left(i\dfrac{p}{2}\dfrac{z}{d}\right) & i = 2k \end{cases} \qquad k = 1,2,3,\ldots$$

Figure 6 shows the temperature histories at the mid-surface of the composite as predicted by COMPRO and the super element technique. Note that convergence of the finite element results is achieved with ten 4-noded isoparametric elements through the thickness while in the proposed super element method the number of analytical terms that is used within each time step is adaptively controlled throughout the analysis. This is shown graphically in **Figure 6** where it can be seen that during the exothermic reaction a maximum of 11 terms in the series is required to capture the steep temperature gradient leading up to the peak temperature but at all other times the number of terms needed are considerably less. **Figure 6** also shows that during this critical phase of the process cycle, the time step size for numerical integration has to be significantly reduced to maintain solution accuracy. This applies to both the finite element and super element methods identically.

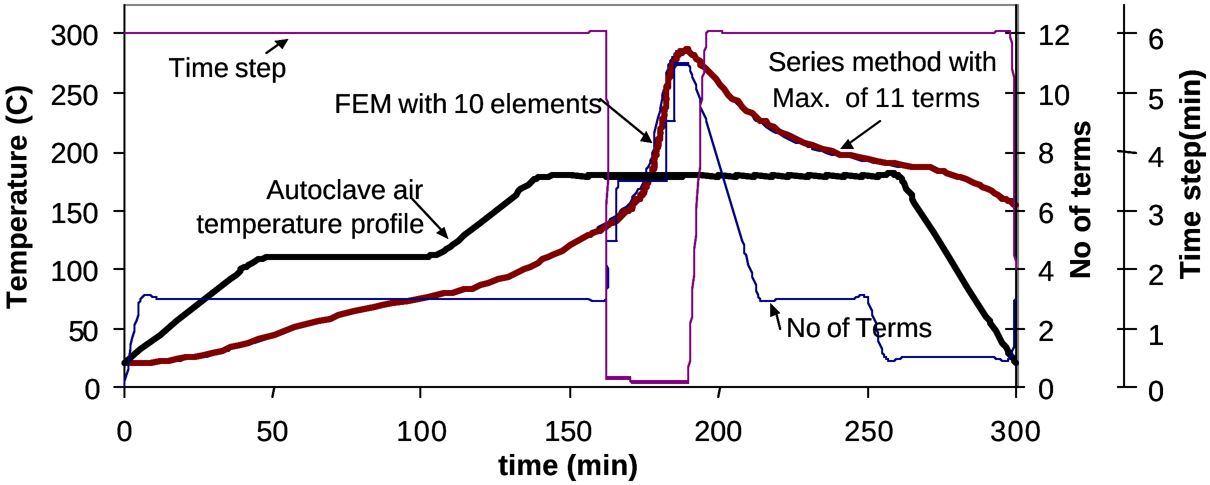

Figure 6 *Temperature histories at the mid-surface of the composite part as predicted by COMPRO and the super element technique. Also shown is the variable number of analytical terms as well as the time step used in the super element method during the process cycle.*

Clearly in the finite element method we need to generate a full 2D mesh, then refine it and run the code a number of times to ensure that convergence is achieved. In so doing, the number of elements that are to be used throughout the analysis are fixed and dictated by the rather fine mesh that is often needed to capture rapid changes in temperature. The advantage of using analytical terms in the direction where rapid changes in temperature and degree of cure are expected is that these terms can be judiciously added or dropped as needed without having to re-mesh. The net result is a significant saving in complex mesh generation and computational run times.

CONCLUSIONS

It has been shown elsewhere that a CHILE/PVE formulation is theoretically equivalent to a VE model for constitutive modeling of composite materials undergoing curing for many conventional cure cycles. Here we present a numerical case study that shows very good agreement between the VE and PVE predictions in a one-dimensional case. Because of the correlation of time and frequency based PVE formulations, both can be used in modeling. PVE formulations are significantly more efficient and easier to implement than VE formulations and there is therefore a great incentive to use them.

In addition, a super element approach is introduced that removes the necessity of through thickness meshing and is computationally more efficient than the conventional finite element method in capturing the details of the temporal distribution of temperature in a curing composite part. The number of terms required in the super element method can change dynamically during the computation and increase only when necessary.

REFERENCES

[1] R.H. Nelson and D.S. Cairns,. ‘Prediction of dimensional changes in composite laminates during cure’, *Proc. 34th International SAMPE Symposium*, May 8-11, 1989, pp. 2397-2410.

[2] A. Johnston, R. Vaziri, and A. Poursartip, ‘A plane strain model for process-induced deformation of laminated composite structures’, *J. Composite Materials*, **35**(16), pp. 1435-1469, 2001.

[3] Y.K. Kim, and S.R. White, ‘Stress relaxation behaviour of 3501-6 epoxy resin during cure’, *Polymer Engineering and Science*, **36**(23), pp. 2852-2862, 1996.

[4] D. Adolf, and J.E. Martin, ‘Calculation of stresses in cross-linking polymers’, *Journal of Composite Materials*, **30**(1), pp. 13-34, 1996.

[5] Z. Manko, ‘Thermal analysis of engineering structures by the finite strip method", *Canadian Journal of Civil Engineering*, **13**, pp. 761-768, 1986.

[6] Y.K. Malikov, V.G. Isienko, and A.E. Ostrotin, ‘Construction of super elements for heat-conduction and potential problems’, *Journal of Macromol. Sci. - Chem.*, **55**(6), pp. 1444-1450, 1989.

[7] N. Zobeiry, R. Vaziri and A. Poursartip, ‘An Efficient Pseudo-Viscoelastic Model for Evaluation of Residual Stresses in Thermoset Composites During Cure’, manuscript to be submitted to *J. Composite Materials*, 2003.

[8] A. Rasekh and R. Vaziri, ‘An Efficient Super Finite Element Model for the Thermo-Chemical Analysis of Composites During Manufacturing’, manuscript to be submitted to *Int. J. Numer. Meth. Engng*, 2003.