PROCESSING-INTERPHASE RELATIONSHIPS FOR THE CURING OF THERMOSETTING-MATRIX COMPOSITES

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ABSTRACT

Fabrication of thermosetting-matrix composites is based on a critical step of cure, which involves applying predefined temperature cycle to a fiber-resin mixture. Several mass transport processes occur in the vicinity of the reinforcement fiber, leading to the formation of an interphase region with different chemical and physical properties from the bulk resin. The cure cycle applied on the macroscopic boundaries of the composite govern the microscopic cure kinetics near the fiber surface, which, in turn, determines the interphase evolution with time, and the life and properties of the composite. Current studies in the literature mostly focus on the macroscopic thermochemical processes, and the linkage between the cure cycles and the interphase structure evolution has not been rigorously studied. A multiscale thermochemical model is presented in this paper to provide the critical link of relating the process parameters to the interphase formation, which is essential for optimizing cure cycles to obtain tailored interphase in composite materials.

KEY WORDS: Polymer Matrix Composites, Process Modeling, Interphase Kinetics, Curing of Polymers

1. INTRODUCTION

During the cure of thermosetting polymer composites, the presence of reinforcing fibers significantly alters the resin composition in the vicinity of the fiber surface via several microscale processes, forming an interphase region with different chemical and physical properties from the bulk resin. The interphase resides in a region between the original constituents of the composite with a size of one to a few thousand nanometers (1–4). The performance of the composite is determined by the ability of the matrix to transfer load to the reinforcing fiber, and is thus controlled by the interphase region. The structure and properties of the interphase are the dominant factors governing the overall composite properties and performance.

The studies in the literature on interphase have focused primarily on the experimental determination of the influence of interphase on the mechanical behavior of the composite
materials (2–5, for example). Fiber surface modifications such as high temperature treatment and sizing, are commonly implemented to tailor the structure of the interphase regions and to investigate their effects on the mechanical and other properties of the composite materials. Due to complexities of the molecular level mechanisms that occur in the vicinity of the fibers during the process, prediction of the interphase evolution as function of processing parameters has been the subject of little attention.

Palmese (1) presented a model for predicting the interphase composition profile under thermodynamic equilibrium conditions of a non-reacting epoxy-amine resin system. The principle of minimum free energy was invoked to set up the equilibrium state, accounting for enthalpy interaction between fiber surface and resin components, and the calculation of Gibbs free energy was based on a Flory-Huggins type lattice structure. Hrivnak (6) extended Palmese's model to a reacting system by using renewal theory models to the construction of the assembly Gibbs free energy and the associated chemical potential. In an alternative approach, a kinetics-based description of the governing phenomena was developed by the authors to predict the interphase development during thermosetting composite processing (7–10). In this method, mass conservation principle was employed to describe the transport processes of multilayer adsorption, desorption and diffusion near a fiber surface, which are accompanied by simultaneous cure reaction between the resin components. The time evolution of interphase concentration profile gradients before the gelation of the thermosetting system was predicted as function of material and process parameters.

The models of interphase formation consider a microscale domain near a fiber surface, and the temperature is assumed to be known. In a simulation of the cure of thermosetting composites, however, the temperature filed must be computed from the energy equation to predict the temperature history at different locations in the material. The solution of the energy equation needs the information of interphase cure kinetics, consequently, the energy equation and the cure kinetics equations are coupled. No study has been reported in the literature to directly link the cure cycles to the interphase kinetics, and this paper is aimed to fill the critical void. A multiscale thermochemical model is developed in the next section, which couples the macroscale energy equation with the microscale interphase cure kinetics equations. The evolution of interphase concentration profiles is presented at various locations of the composite for two selected cure cycles.

2. MULTISCALE THERMOCHEMICAL MODEL

In this study, the geometry of the composite is considered to be cylindrical, which corresponds to a die of circular cross section, in a pultrusion process (11–13). However, the model development and relevant results are readily extended to the other geometries involved in the manufacturing techniques such as autoclave molding and liquid molding. In a pultrusion process, the resin-fiber mixture is pulled through a long heated die with prescribed temperature variation. The elevated temperatures initiate an exothermic crosslinking cure reaction among the species in the resin, which transform the soft initial mixture entering the die to a hard product at the die exit. The dominant physical and chemical phenomena are: (a) the heat transfer associated with the heating of the composite, and (b) the chemical reaction leading the cure process (11–13).
The heat transfer inside the pultrusion die is considered to be one dimensional radially, at steady-state, and with a source term reflecting the reaction heat of the cure process. The Lagrangian form of the heat equation for a composite cross-section may be written as (11):

\[
\frac{\partial}{\partial t} \left( \rho_{f} c_{p} T \right) = \frac{1}{r} \frac{\partial}{\partial r} \left( k_{r} r \frac{\partial T}{\partial r} \right) + C_{E0} \Delta H_{f} (1 - v_{f}) \frac{\partial \varepsilon}{\partial t} \tag{1}
\]

where the variables \( t \) and \( r \) are the Lagrangian time and radial coordinate, respectively, \( \Delta H_{f} \) is the heat of the cure reaction, \( C_{E0} \) is the initial concentration of the epoxy resin at the die entrance, \( v_{f} \) is the fiber volume fraction, and \( T \) is the local temperature of the mixture. The three material properties, namely, the thermal conductivity, \( k \), the density, \( \rho \), and the specific heat, \( c_{p} \), are evaluated based on the weight fraction of the fiber-resin mixture (11). The term \( \partial \varepsilon / \partial t \) is the local reaction rate, and its determination is the focus of the remaining discussion in this section.

The cure reaction rate is commonly modeled by empirical correlations, which are obtained by using data from the bulk reactions with uniform mixing of the reacting species in the absence of the reinforcing fibers (11). The presence of fibers, however, has been found to cause concentration gradients in the vicinity of the fiber surfaces through the preferential adsorption mechanism (7–10). Consequently, the reaction kinetics is significantly changed by the spacial variation of the stoichiometric ratio, i.e., the non-uniform mixing of the reacting species. A model of the microscale cure kinetics near the fiber surfaces has been developed by the authors (7–10), and is adopted in this paper to determine the cure reaction rate, \( \partial \varepsilon / \partial t \).

The geometry considered in the cure kinetics model is the inter-fiber space in a composite having a typical staggered fiber arrangement [Figure 1(a)]. The domain in the model development is idealized as the region between two identical infinite planes representing the fiber surfaces [Figure 1(b)], which may be justified by the fact that the interphase thickness is often small in comparison to the fiber diameter. A graphite fiber/epoxy-amine thermosetting system is considered in the model development; however, all the derivations and results are applicable to a general two-component thermosetting system. The domain between the two fiber surfaces is

![Figure 1](image1.png)

![Figure 2](image2.png)

Figure 1: (a) A representative fiber arrangement in the composite, and (b) schematic of the domain between two fiber surfaces considered in the modeling.

Figure 2: Schematic of the adsorption, desorption, and diffusion processes in an epoxy-amine system.
further divided into molecular layers where one molecule of epoxy or amine can occupy only one of these layers, and $N_L$ is the total number of molecular layers in the half domain (Figure 2).

Due to the interaction between resin molecules and the fiber surface, as well as those among resin molecules themselves, epoxy and amine molecules can move from layer to layer. The solid surface can adsorb molecules from a “bulk” state into an “adsorbed” state, and conversely, molecules in the “adsorbed” state may be desorbed into the “bulk” state. Molecules in the “adsorbed” state are treated to be fixed in the space and are not permitted to diffuse, while molecules in the “bulk” state may diffuse within the resin mixture. Figure 2 shows the molecular layers in the model domain, where the adsorption layers contain molecules in the “adsorbed” state, while the bulk layers hold molecules in the “bulk” state. Although the adsorption and bulk layers are drawn separately to illustrate the mass exchange between the “adsorbed” and “bulk” states, the corresponding layers essentially occupy the same space, i.e., the $(i)$th adsorption layer and the $(i)$th bulk layer are overlapped. Chemical reaction between epoxy and amine happens simultaneously during the adsorption, desorption and diffusion processes, resulting in a continuously evolving concentration profile that is “frozen” in space upon gelation of the thermosetting system.

The mass balance analysis for the epoxy molecule in any $(i)$th adsorption layer in Figure 2 yields

$$
\frac{dN_{E,i}}{dt} = \left( R_{a,E}(i-1,i) + R_{a,E}(i,i) + R_{a,E}(i+1,i) \right) - \left( R_{d,E}(i-1,i) - R_{d,E}(i,i) - R_{d,E}(i+1,i) - R_{r,E}(i) \right)
$$

(2)

In Eq. (2), $\frac{dN_{E,i}}{dt}$ is the rate of change of total number of epoxy molecules in the $(i)$th adsorption layer, and the subscripts $E$ and $i$ denote epoxy and $(i)$th layer, respectively. Epoxy molecules in the “bulk” state in the $(i-1)$th, $(i)$th, and $(i+1)$th layers may be adsorbed into the $(i)$th molecular layer, denoting by the rate terms $R_{a,E}(i-1,i)$, $R_{a,E}(i,i)$, and $R_{a,E}(i+1,i)$ respectively; in a reverse process, the adsorbed epoxy molecules in the $(i)$th layer can also be desorbed into the bulk in the $(i-1)$th, $(i)$th, and $(i+1)$th layers through the rate terms $R_{d,E}(i-1,i)$, $R_{d,E}(i,i)$, and $R_{d,E}(i+1,i)$; further, the depletion of epoxy in the $(i)$th adsorption layer through chemical reaction is determined by the rate term $R_{r,E}(i)$.

Considering the rate of change of the number of epoxy molecules in the “bulk” state in the $(i)$th layer, i.e., $\frac{dN_{E,i}}{dt}$, we may obtain

$$
\frac{dN_{E,i}}{dt} = D_{EA} \frac{N_{E,i-1} + N_{E,i+1} - 2N_{E,i}}{\Delta L} - R_{a,E}(i-1,i) - R_{a,E}(i,i) - R_{a,E}(i+1,i) + R_{d,E}(i,i) + R_{d,E}(i,i+1) - n_1 k_r N_{E,i}
$$

(3)

where $D_{EA}$ is the mutual diffusivity in the binary epoxy-amine mixture, $\Delta L$ corresponds to the physical size of a molecular layer, $n_1$ is the number of moles of epoxy needed to produce one mole product, and $k_r$ is the reaction rate determined by the empirical correlations mentioned above.
The rate terms of adsorption, desorption, and reaction depend on the number of epoxy, amine and product molecules in the adsorption and bulk layers. Similar mass conservation analyses may be applied to the amine and product molecules in the “adsorbed” and “bulk” states, yielding the rate of change equations for the corresponding species. The review of the kinetics model so far paves the way for the development of the thermochemical model in this section, and the readers are referred to refs. (7–10) for details.

The degree of cure, $\varepsilon$, is defined as:

$$\varepsilon = \frac{N_{E0} - N_E}{N_{E0}}$$  \hspace{1cm} (4)

where $N_{E0}$ is the initial number of epoxy molecules in the model domain between two fiber surfaces (Fig. 2), and $N_E$ is the instantaneous number of epoxy molecule in the model domain:

$$N_E = \sum_{i=1}^{N_i} (N_{E,i} + N_{Ew,i})$$  \hspace{1cm} (5)

Differentiating Eqns. (2) and (3) with respective to time yields:

$$\frac{\partial \varepsilon}{\partial t} = \frac{1}{N_{E0}} \frac{\partial N_E}{\partial t} = \frac{1}{N_{E0}} \sum_{i=1}^{N_i} \left( \frac{dN_{E,i}}{dt} + \frac{dN_{Ew,i}}{dt} \right)$$  \hspace{1cm} (6)

where the rates of change, $dN_{E,i} / dt$ and $dN_{Ew,i} / dt$, are given by Eqns. (2) and (3), respectively. The heat equation, Eq. (1), for the macroscale composite domain and the reaction rate equation, Eq. (6), for the microscale model domain in Fig. 2 consist of a multiscale thermochemical model. Note that Eqns. (1) and (6) are coupled through the temperature dependence of the rate terms in Eqns. (2) and (3).

Two boundary conditions and an initial condition are invoked for Eq. (1): (I) the temperature at the outer radius of the composite material corresponds to the temperature of the die wall (or the prescribed cure cycle), $T_c(t)$, (II) symmetric conditions exist at the centerline of the die, and (III) the initial temperature at the die entrance is specified to be $T_i$. The initial conditions for Eqns. (2), (3), (6) and the rate equations for the other species are: (IV) the number of molecules of each species in the “adsorbed” state is zero, and (V) the number of product molecules is zero, and all the resin molecules are in the “bulk” state (7–10). The above five conditions may be expressed mathematically as:

(I) $T (R_o,t) = T_c (t)$; (II) $\partial T / \partial r (0,t) = 0$; (III) $T (r,0) = T_i$

(IV) $N_{E,i} = N_{A,i} = N_{P,i} = 0$; $(i = 1,2,\cdots N_L)$

(V) $N_{Pw,i} = 0$; $N_{Ew,i} = N_{E,0}$; $N_{Aw,i} = N_{A,0}$; $(i = 1,2,\cdots N_L)$  \hspace{1cm} (7)

The governing equations, Eqns. (1) and (6), along with the boundary and initial conditions, Eq. (7), were solved numerically using an implicit finite-difference scheme with a control volume formulation (9). The mesh for the macroscopic composite domain contained 64 numerical grids along the radius direction, and the time step $\Delta t$ was determined such that the mesh Fourier number $k \Delta t / \rho c_p \Delta r^2$ is less than unity. Depending on the fiber volume fraction, each computational grid may consist of a large number of representative volume elements (RVE) shown in Figure 2. All the RVEs in a grid experience the same temperature history, and hence, the same concentration profile evolution history. Within each time step, the temperature field
obtained from Eq. (1) is used to calculate the cure reaction rate \( \frac{d\varepsilon}{dt} \) in Eq. (6), which, in turn, is substituted into Eq. (1) to update the temperature field; and the procedure is performed until the temperature field is converged. The ordinary differential equations [e.g., Eqns. (2) and (3)] were solved by a fourth order Runge-Kutta method (7–10). The stopping criterion for the numerical simulation is that all the sections of the composite reach the gelation point, which corresponds to \( \varepsilon = 0.6 \).

3. RESULTS AND DISCUSSION

The thermochemical model developed in the previous section is used to calculate the molar concentration of the resin component as a function of the molecular layers at different locations in the composite for various cure cycles. A nondimensional form of the heat equation, Eq. (1), and its boundary and initial conditions is obtained by introducing the dimensionless temperature, location, and time in the radius direction as:

\[
\theta = \frac{T - T_0}{T_0}, \quad r = \frac{r}{R_0}, \quad t' = k_{d,E} e^{-E_a / RT_0} t,
\]

where \( T_0 \) is the reference temperature; while the dimensionless form of the reaction rate equation, Eq. (6), and its initial conditions is derived by introducing a dimensionless time \( t' \) and dividing all the number of molecules (e.g., \( N_{E,i}, N_{A,i} \)) by the initial number of epoxy molecules in the layer next to the middle plane \( N_{E,0} \) (e.g., \( N'_{E,i} = N_{E,i} / N_{E,0} \)).

The principal dimensionless groups that govern the interphase concentration evolution at various locations in a composite are identified as follows: (1) the adiabatic reaction temperature \( \theta_{ad} = \Delta H_r C_{Eo} (1 - v_f) / \rho c_p T_0 \), (2) dimensionless epoxy adsorption energy, \( E^*_{a,E} = E_{a,E} / RT_0 \), (3) dimensionless epoxy desorption energy, \( E^*_{d,E} = E_{d,E} / RT_0 \), (4) epoxy diffusion ratio \( \beta_{E} = k_{d,E} e^{-(E_{d,E}-E_{a,E}) / RT_0} / k_{a,E} \), (5) epoxy diffusion ratio \( \phi_{EA} = \frac{D_{EA} e^{E_{a,E} / RT_0}}{\Delta T^2 k_{a,E}} \), (6) dimensionless amine adsorption energy, \( E^*_{a,A} = E_{a,A} / RT_0 \), (7) dimensionless amine desorption energy, \( E^*_{d,A} = E_{d,A} / RT_0 \), (8) amine desorption ratio \( \beta_{A} = k_{d,A} e^{-(E_{d,A}-E_{a,A}) / RT_0} / k_{a,A} \), (9) amine adsorption ratio \( \alpha_{A} = k_{d,A} e^{-(E_{d,A}-E_{a,A}) / RT_0} / k_{a,A} \), and (10) adsorption Damköhler number \( \gamma = k_{d,E} e^{E_{a,E} / RT_0} / k_{a,E} \). In this study, the number of molecular layers in the model domain is kept fixed at \( N_L = 100 \), the reference temperature is kept at \( T_0 = 80^\circ C \), and the outer radius of the composite \( R = 0.00635m \). Furthermore, the cure cycles begin with a linear ramp from \( \theta_i = -0.33 \) to \( \theta_f = 0.50 \) within ramp time \( \Delta t'_{ramp} \), followed by a hold stage with a constant temperature \( \theta_f \).

Figures 3(a)–(f) present the distributions of the number of epoxy and amine molecules within a microscopic representative volume element (shown in Figure 2) at different nondimensional times during the process. The results correspond to a cure ramp time \( \Delta t'_{ramp} = 80 \), and the location of the RVE is at the centerline of the composite, i.e., \( r/R=0.0 \). Although the total concentrations are the most relevant to the composite material properties, the results of the adsorbed and bulk fractions are presented as well to better elucidate the trends in the total concentration development. Figures 3(a) and 3(b) present the concentration profiles for the molecules in the adsorbed state; Figures 3(c) and 3(d) correspond to bulk state concentration profiles; and Figures 3(e) and 3(f) show the total concentrations of epoxy and amine, \( N'_{E,tot} \) and \( N'_{A,tot} \). The following parameter combination is employed: \( \theta_{ad} = 0.072, E^*_{a,E} = E^*_{a,A} = 3.4, E^*_{d,E} \).
= E^*_{d,E} = 6.8, \gamma = 0.01, \beta_E = 0.75, \alpha_A = 1.5, \beta_A = 0.75, N'_E,0 = N'_A,0 = 1, N'_0 = 1, (N'_0 = N_0/N_{E,0}, where N_0 is the number of adsorption sites at the fiber surface) and \phi_{EA} = 6.0. The desorption ratios \beta_E and \beta_A are chosen to be relatively small which indicates that the resin molecules are easily adsorbed onto the fiber surface.

Figure 3: Interphase concentration profiles at the centerline, in terms of relative number of (a) epoxy molecules and (b) amine molecules in the adsorbed state; (c) epoxy molecules and (d) amine molecules in the bulk state; (e) total epoxy molecules and (f) total amine molecules in both states, as a function of the molecular layer at four different times during the cure process.

In the adsorbed state profiles, Figures 3(a) and 3(b), the number of molecules for both of the species increase monotonically from \( t' = 0.11 \) to \( t' = 54.00 \) due to adsorption onto the surface, resulting in a high concentration region near the fiber surface; at the gelation time \( t' = 137.43 \),
however, the reactant concentrations in the vicinity of the fiber surface decrease due to chemical reaction. The concentration profiles are seen to propagate from a small region near the fiber surface at \( t' = 0.11 \) to the far region at the gelation time, which is identified as a strong adsorption effect. The number of epoxy molecules near the fiber surface is smaller than that of the amine molecules owing to the larger amine adsorption rate \( (\alpha_A = 1.5) \). The adsorption/desorption processes cause the deficit of species in the bulk state near the fiber surface, as shown in Figures 3(c) and 3(d) from \( t' = 0.11 \) to \( t' = 54.00 \). However, the diffusion process compensates for the deficit at the gelation time, \( t' = 102.0 \), when the concentration gradients in the bulk state approach zero. The total concentration profiles of each species [Figures 3(e) and 3(f)] show minima at \( t' = 0.11, t' = 10.80 \) and \( t' = 54.00 \), which can be explained by the coupled influence of the adsorption/desorption and the diffusion processes as discussed above.

![Figure 4](image-url)

**Figure 4:** Total interphase concentration profiles for (a) epoxy and (b) amine molecules near the middle point; (c) epoxy and (d) amine molecules near the outer radius. The results correspond to cure ramp time \( \Delta t'_{\text{ramp}} = 80 \), and a strong adsorption effect.

Figures 4(a)–(d) present the total concentration evolution at two other locations in the composite, i.e., the middle point, \( r/R = 0.5 \), and the outer radius \( r/R = 1.0 \); the cure ramp time and other parameters retain the values as in Figure 3. Since resin materials at larger radius experience higher temperatures, the gelation time decreases from \( t' = 137.43 \) at the centerline to \( t' = 120.53 \) at the middle point [Figures 4(a) and (b)], and \( t' = 75.65 \) at the outer radius [Figures 4(c) and (d)]. All the concentration profiles show minima before the gelation time, which may be explained by the same arguments in Figure 3. At different locations in the composite, the final concentration profiles show significant deviations from each other. In Figures 4(a) and (b), the concentration
gradients at the gelation time become zero between layers 80 and 100, while in Figures 4(c) and (d) the zero gradient region is extended between layers 60 and 100. A smaller zero gradient region is observed in Figures 3(e) and (f). At larger radius, less time (i.e., the gelation time) is available for the concentration gradient to propagate from the fiber surface to the far region, hence the increase in the zero gradient region.

Figure 5: Total interphase concentration profiles for (a) epoxy and (b) amine molecules near the centerline; (c) epoxy and (d) amine molecules near the middle point; (e) epoxy and (f) amine molecules near the outer radius. The results correspond to cure ramp time $\Delta t'_{\text{ramp}} = 80$, and a weak adsorption effect.

Figures 5(a)–(f) show the total concentration profiles at three locations in the composites, and the results pertain to the parameter combination of $\beta_E = 1.5$, $\alpha_A = 0.5$, and $\beta_A = 2.0$; the cure ramp time and all other parameters retain the values as in Figure 4. The concentration profiles in the
adsorbed state (omitted here for brevity) growth from $t' = 0.11$ to $t' = 10.80$, and remains invariant afterwards. An equilibrium state is thus reached, where the desorption and adsorption processes balance each other and the influence of the fiber surface only propagate to a few molecular layers. By increasing $\beta_A$ and $\beta_E$, and decreasing $\alpha_A$, the desorption process is strengthened with respect to adsorption, which corresponds to a relatively weak “force field” by the fiber surface that can only penetrate into a few molecular layers. The gelation times at different locations in Figure 5 are identical to the corresponding values in Figures 3 and 4, which

![Figure 6: Total interphase concentration profiles for (a) epoxy and (b) amine molecules near the centerline; (c) epoxy and (d) amine molecules near the middle point; (e) epoxy and (f) amine molecules near the outer radius. The results corresponds to cure ramp time $\Delta t_{\text{ramp}} = 160$, and a strong adsorption effect](image)

is caused by the first order cure kinetics adopted in this study. Since only the concentration of the epoxy (instead of the concentrations of both reactants) is considered in the first order kinetics,
different concentration profile evolutions in the microscale domains do not influence the overall reaction rate in the composite domain. An improved cure kinetics model will be implemented in a future work for a more realistic simulation. The equilibrium profiles in the absorbed state were developed at time $t' = 10.80$, which is before all the gelation times at different location, consequently, the final concentration profiles in Figure 5 are almost identical.

Figure 7: Total interphase concentration profiles for (a) epoxy and (b) amine molecules near the centerline; (c) epoxy and (d) amine molecules near the middle point; (e) epoxy and (f) amine molecules near the outer radius. The results correspond to cure ramp time $\Delta t'_{\text{ramp}} = 160$, and a weak adsorption effect.

The results corresponding to a longer cure ramp time $\Delta t'_{\text{ramp}} = 160$ are shown in Figures 6 and 7, which follow the presentation format in Figure 5(a)–(f). Figure 6 retains the parameter combination in Figure 3 (or 4). However, the gelation times in Figure 6 are longer than the
corresponding cases in Figures 3 and 4 due to lower cure temperatures, e.g., an increase is found from $t' = 137.47$ in Figure 3(e) to $t' = 168.21$ in Figure 6(a). Consequently, the final concentration profiles are also changed for different cure cycles, and smaller nonzero gradient regions are observed in Figure 6 than the corresponding cases in Figures 3 and 4. Note that the final concentration profiles in Figures 6(a) and 6(c) [or in Figures 6(b) and 6(d)] are identical, which may be explained by the fact that the adsorption/desorption equilibrium states were achieved before the gelation times. Figure 7 has the same parameter combination in Figure 5, and the effect of different cure cycles and locations in the composites are negligible since all the gel times are longer than the adsorption/desorption equilibrium time.

The influence of other parameter combinations and cure cycles on the concentration profile evolution can be discussed in similar ways and detailed discussion will not be included in the paper. The predicted interphase composition profiles at different locations of the composites are important input data to the prediction of overall composite material properties (1, 14). The results presented in this section may be used to select the cure cycles for desired interphase structure.

4. CONCLUSIONS

A microscale kinetics model of interphase formation is coupled with a macroscale energy equation to simulate the cure process of thermosetting composite material. The final concentration gradient caused by the adsorption-desorption process may vary at different locations in the composites, which experience different temperature history. It is shown that the composition profile changes significantly before the adsorption/desorption equilibrium time, but remains constant afterward. Consequently, the effect of cure cycles and locations in the composite may be negligible when gelation times are always longer than the adsorption/desorption equilibrium time in the whole composite domain.

5. ACKNOWLEDGEMENT

The work reported in this paper was carried out as part of the MEANS program funded by the Air Force Office of Scientific Research (Grant No. F496200110521). We are grateful for their support.

6. REFERENCES