COMPUTATIONAL MECHANICAL ANALYSIS OF COMPOSITE BONDLINES UNDER ENVIRONMENTAL MOISTURE LOADS

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Abstract. A combined moisture diffusion and mechanical computational analysis methodology was developed as part of an independent research program at Lockheed to enhance our understanding of nonlinear and coupled physical processes in materials. The physical behavior of interest is the mechanical response of composite material systems to environmental conditions which can change the materials' moisture content. In particular, it is desirable to know what set of environmental conditions will affect the integrity of a partial adhesive bondline when a bondline gap (no adhesive) is present. The Lockheed proprietary finite element analysis code DIAL was modified to analyze this phenomena in two stages. First, the temporal moisture partial pressures in the materials are calculated from initial and environmental boundary conditions and second, these partial pressures are then passed to a quasi-static mechanical analysis where the moisture data at each time step is treated as a dilatation (swelling) load. The resulting stress and strain state is then calculated, as well as gap closure, if any.

Demonstration of this methodology was on a relatively simple 2-dimensional axisymmetric example problem. The results show primarily compressive stresses caused by the positive dilatation (swelling) induced by moisture intrusion of the structure. The stresses concentrate at adhesive bondlines, and bondline gap behavior (i.e., the absence of a contiguous adhesive bond at material interfaces) is correctly simulated. It should be noted that the behavior of the gap and any resultant stress/strains due to a change in moisture is problem dependent, and this example problem is meant as a demonstration of methodology.

INTRODUCTION

The increasing use of composite materials in aerospace systems can lead to unexpected effects by responding to various environmental factors. Composite material systems are often joined with adhesives which transmit structural loads from one adherend material to another. Because these materials respond to changes in environmental conditions during storage, deployment and operation, the system designer must investigate and assess the structural response produced by these changes in the environment. The analyst must then examine the effect of these changes on materials where the adhesive bondline is either absent (gaps), or partially failed. It is conceivable that the gaps might play an important role in the response of the remaining adhesive to various environments and their ability to carry additional applied loads (accelerations, static and dynamic external forces). Environmental effects on adhesive systems are often dismissed as secondary to the applied loads, yet as this study shows, these environmental loads can produce significant stress and strain fields.

This study investigates the physics of coupled moisture diffusion and mechanical dilatation in adhesively bound composite assemblies. Additional computational abilities within the chosen finite element code were developed to examine these phenomena. Since composites exhibit highly directional (anisotropic) physical properties, both in mass transport and mechanical characteristics, the computational methodology must be robust enough to include these properties. Nonlinearities in the adhesive properties, such as changes in elastic modulus versus moisture content, can also be included.

METHOD

The complexity of simulating coupled physical processes requires the use of a general purpose finite element code capable of linking data bases from each separate analysis. The DIAL code is structured in a modular and database architecture that allows separate analyses to be linked. This code also allows material nonlinearities and anisotropy for full characterization of the composites and adhesives. It is also capable of simulating the physics of material contact through the use of gap elements; that is, elements with zero stiffness when the gap is open and a large stiffness when the gap closes back to zero. These characteristics properly simulate a gap which does not transfer loads when open, and which does not allow the interpenetration of material boundaries when the gap is closed. The analysis of bondline gap closure and load transfer across a zero gap is required in the simulation of material systems whose dilatation can create internal stresses when bondline gaps close.

The method of analysis of this coupled system in this context is simple. Local equilibrium is assumed to exist between the moisture concentration and the stress/strain state. Also assumed is coupling in one direction only - transient moisture diffusion to mechanical response. Implicit in this assumption is that the material dilatation due to moisture transport (i.e., changes in moisture concentration) creates the mechanically strained state, and that the stress and strain state does not affect the rate of moisture transport or its solubility. Next, computationally solve (independent of stresses and strains) for the spatial and time moisture concentration maps subject to initial and boundary limitations at a constant, uniform temperature. If local equilibrium is assumed, then the mechanical response is quasi-static only and responds to moisture concentration changes on the same time scale as the moisture diffusion process. Hence, the coupling is loose, or sequential. The DIAL code will allow full coupling, where the stress/strain state of the material affects its moisture transport rate and equilibrium level. This requires a constitutive law and experimental data characterizing the reverse coupling.

A restriction of this methodology is that it is limited to small mesh distortions caused by solute swelling or contraction. This is a physical as well as a computational requirement. Physically, if the material deformations are large, the moisture gradients and concentration change spatially, and hence, are tightly coupled to the mechanical analysis. In practice, the moisture concentrations in structural composites and material deflections are small (<1 percent by wt.) even at high humidities. Computationally, two finite element grids are required - one each for the moisture diffusion and mechanical analysis. These two grids must spatially superimpose (within a chosen tolerance) at the nodal locations in order to transfer the moisture data to the mechanical model as loads.

Moisture Transport Analysis

The moisture diffusion in a composite material is based on an analogy to the process of heat conduction in a solid. In this way, we can take advantage of finite element solvers written for heat conduction and apply the same solvers to diffusional mass transport.

Assuming a single species i (water) can dissolve in a polymer matrix, and the process of mass transport is characterized by Fick's first law of diffusion and no convection exists, then the pointwise mass balance can be shown to be (Bird, 1960; Slattery, 1981):

$$\frac{\partial C^{(i)}}{\partial t} = \nabla \cdot (D^{(i)} \cdot \nabla C^{(i)}) + R^{(i)} \qquad (1)$$

where $D^{(i)}$, $C^{(i)}$, and $R^{(i)}$ are the mass diffusivity tensor, species mass concentration and volumetric mass source, respectively, and species i does not react with itself or any other species including the polymer, where t is time and ∇ is the gradient operator. If we assume there is no volumetric source term ($R^{(i)} = 0$), the process of mass transport is ideally reversible. The use of concentration as the unknown quantity in Eq. (1) presents a problem when two polymers are joined (fused) at an internal boundary and have different solubilities for species i at a given, fixed temperature. The concentration, $C^{(i)}$, can be discontinuous across an internal boundary σ, as illustrated in Fig. 1, although the appropriate boundary condition at an internal interface is given by a mass flux continuity condition, or jump balance at σ for species i:

$$\left[\left| q^{(i)} \cdot n^{(i)} \right|\right] + r^{\sigma} = 0 \qquad (2)$$

and where $D^{(i)}_{1,2}$ are the mass diffusivities for adjacent polymers numbers 1 and 2,

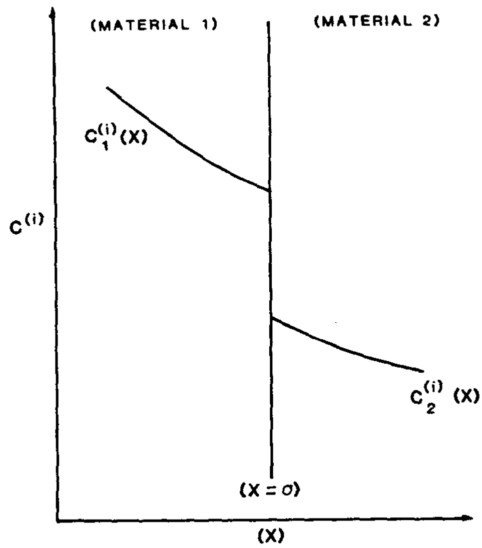


Fig. 1. Discontinuity of concentration of species i at an internal interface (σ).

$$\text{where } \left[\left| q^{(i)} \cdot n^{(i)} \right|\right] = -D_1^{(i)} \cdot \frac{\partial C^{(i)}}{\partial n}\bigg|_{\sigma} \cdot n + D_2^{(i)} \cdot \frac{\partial C^{(i)}}{\partial n}\bigg|_{\sigma} \cdot n \qquad (3)$$

respectively and q and n are the mass flux and outward pointing unit normal vectors, respectively, and r is the rate of creation of species i.

No analog to this situation exists for heat conduction across an internal boundary, because the temperature (T) is continuous across σ. So the concentration of species i must be converted to another scalar variable which is continuous on σ. If one assumes that a solubility relation exists between the partial pressure of a vapor of species i above a polymer which, at equilibrium, results in a concentration of species i dissolved in the polymer, then in general, one can assume a solubility relation of the form:

$$C^{(i)} = S^{(i)} P^{(i)} \qquad (4)$$

where the solubility coefficient ($S^{(i)}$) can be a function of the solute partial pressure, $P^{(i)}$. But Eq. (4) relates only the external vapor partial pressure $P^{(i)}$ to the concentration of dissolved vapor in the polymer. If we make the assumption that the solute pressure $P^{(i)}$ exists in the polymer, and is also characterized by Eq. (4), then by substitution of Eq. (4) into (1) yields:

$$\xi^{(i)} \frac{\partial P^{(i)}}{\partial t} = \nabla \cdot \left((D^{(i)} \xi) \cdot \nabla P^{(i)} \right) + R^{(i)} \qquad (5)$$

$$\text{where } \quad \xi^{(i)} = S^{(i)} + P^{(i)} \zeta^{(i)} \qquad (6)$$

$$\text{and } \quad \zeta^{(i)} = \frac{\partial S^{(i)}}{\partial P^{(i)}} \qquad (7)$$

where ξ and ζ are the nonlinear solubility function and the non-ideal part of the nonlinear solubility function, respectively.

From hereon the species superscript i will be assumed. If one now compares Eq. (5) to the heat conduction equation, the analogy becomes apparent:

$$\rho C_p \frac{\partial T}{\partial t} = \nabla \cdot (\kappa \cdot \nabla T) + \Phi \qquad (8)$$

where ρ, C_p, T, κ, and Φ are the mass density, heat capacity at constant pressure, temperature, thermal conductivity tensor and volumetric heat source, respectively, as pointed out in previous work by Slattery (1981).

The physical behavior of pressure across a material interface is one of pressure continuity, analogous to temperature. For completeness, the boundary and initial conditions must also be analogous. A prescribed temperature and a prescribed pressure on an external boundary (Γ) are analogous boundary conditions; a convective boundary layer is also of the same form (Slattery, 1981):

$$\left(-D\zeta \cdot \frac{\partial P}{\partial n}\bigg|_{\Gamma}\right) \cdot n = k'(SP|_{\Gamma} - C_{\infty}) \qquad (9)$$

for mass transport

$$\left(-\kappa \cdot \frac{\partial T}{\partial n}\bigg|_{\Gamma}\right) \cdot n = h(T|_{\Gamma} - T_{\infty}) \qquad (10)$$

for heat transport

where k', h and κ are the mass and heat film transfer coefficients and the thermal conductivity tensor, respectively and C_∞ and T_∞ are the respective mass concentration and temperature in a well-mixed fluid surrounding the polymer body.

Only radiant heat transfer on external boundaries does not have an analog in mass transport.

Two simple forms of the constitutive relation between pressure and concentration have been considered by Hopfenberg (in Haward, 1973) and others (Denbigh, 1966); (1) a linear solubility and (2) nonlinear relation.

(1) Linear solubility: S = constant, which implies $\zeta = 0$ and $\xi = S$. This is the one considered for the example analysis.

(2) Nonlinear solubility: S = S(P).

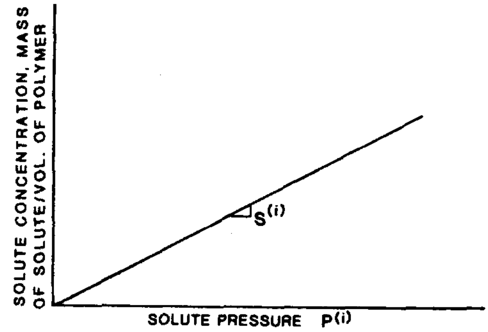
A typical form of the nonlinear relation is:

$$C = \kappa_D^* P + C_H' bP/(1 + bP) \qquad (11)$$

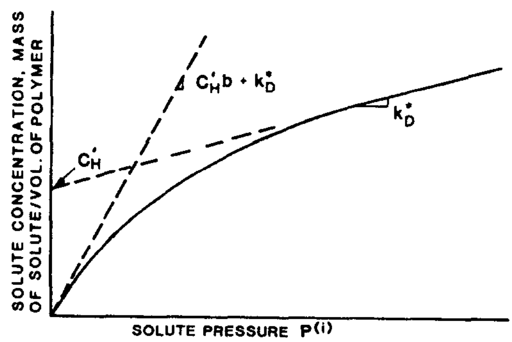
where κ_D^*, C_H', and b are empirical constants. Equation (11) describes a dual-sorption process of dissolved solute and "hole filling". Typical sorption relationships are illustrated in Fig. 2.

The analogy with the thermal conduction is complete, hence, one can see from Eqs. (5) and (7) that the mass diffusion equation can be solved using the standard Finite Element Method for heat conduction, with appropriate parameter substitutions.

For purposes of the present analysis, a simple linear (constant) solubility relation was chosen in lieu of more complete water sorption data. Also, no volumetric sources or sinks, due to chemical reaction, were considered.



2(a): LINEAR, OR HENRY'S LAW SORPTION BEHAVIOR



2(b): NONLINEAR, OR LANGMUIR SORPTION BEHAVIOR

Fig. 2. Empirical relation(s) between species i concentration and pressure, as determined from equilibrium sorption/desorption experiments.

Mechanical Analysis

The mechanical analysis can be divided into two separate areas: the dilatation process and gap analysis. The dilatation, or swelling of the composite materials is due to an uptake of moisture (or shrinkage due to moisture loss). The dilatation process is described by an elastic strain model:

$$\begin{Bmatrix} \epsilon_R \\ \epsilon_Z \end{Bmatrix} = \Delta C^{(i)} \begin{Bmatrix} \beta_R \\ \beta_Z \end{Bmatrix} \qquad (12)$$

where ϵ, and β are the elastic strain and hygrothermal strain components in two dimensions. The gap analysis accounts for the gaps in the bondline adhesive, due either to partial failure or the initial lack of adhesive during fabrication. Gap closure is a discontinuous process, that is, the gap transmits no load across the gap until closure occurs. When closure occurs, assuming no friction, only normal forces are transmitted across the material interface. The gap element in DIAL is a spring separating adjacent nodes. Before closure the spring stiffness is zero. After closure the stiffness is 100 times the modulus of the stiffest material in the analysis. This discontinuous change of gap spring stiffness does not allow for the penetration of adjacent materials. The discontinuity in stiffness does, however, require a convergent solver scheme to balance the forces at each time-step or load condition.

EXAMPLE PROBLEM

A two-dimensional axisymmetric example problem was devised to examine the simulated physics of mass-transport-induced mechanical deformations and to test the computational methodology. Chosen is an assembly of three polymeric composite materials joined by a 'T' shaped gap as illustrated in Fig. 3. The composite chosen is graphite phenolic, with typical properties derived from the published literature (Ishai, 1982). Subject dimensions were chosen for convenience only, and are summarized with typical material properties and boundary and initial conditions in Table 1.

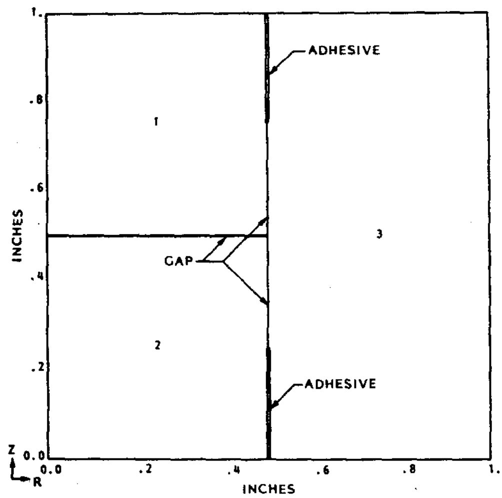


Fig. 3. Example problem geometry axisymmetric composite assembly (numbers in blocks are material numbers - see table 1).

The environmental conditions and mechanical constraints were also chosen for convenience and physical consistency. For example, as Fig. 4 illustrates, the right-hand boundary was sealed to moisture and rigidly fixed (constrained in both the R and Z directions). This is physically consistent because a mechanical attachment of the right-hand boundary to an extremely rigid support would also represent a boundary sealed to moisture transport or flux. The gap represents a particularly difficult

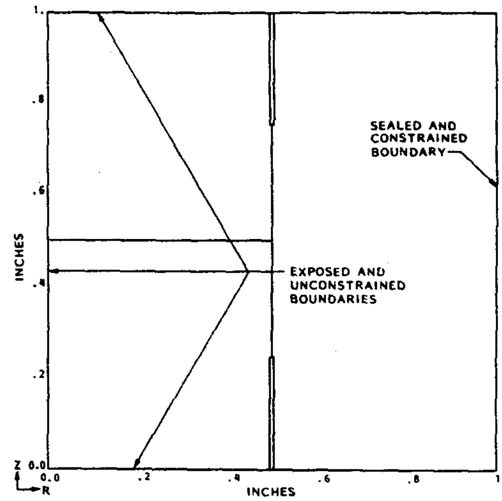


Fig. 4. Example problem boundary conditions.

physical situation with respect to the mass transport of moisture in the air-gap space and absorption into and out of the adjacent materials. For simplicity, the material faces bordering the internal gaps were assumed sealed and not subject to mass flux boundary conditions.

Figures 5 and 6 illustrate the spatial grids for the moisture transport and mechanical analyses, respectively; note that they can be spatially superimposed. The moisture transport model uses linear basis function elements and the mechanical analysis uses quadratic elements. The G's mark the gap elements.

A mass transport analysis was performed to simulate the uptake of moisture and bondline closure over a time period of 50 days. This exposure was to an environmental humidity larger than the initial uniform, equilibrated moisture content of the composite assembly. Figures 7 and 8 illustrate the results of this analysis for days 5 and 50, shown as contours of pressure of water (in atmospheric pressure) in the assembly. The relatively large gradient of pressure on the left-hand boundary is due to the material's typical orthotropic mass diffusivity. Also note the discontinuous pressure contours across the gaps - no transport of moisture across them. These results are typical for a material with constant mass diffusivity and solubility coefficients.

The moisture partial pressure data for each chosen analysis time was transferred to the mechanical model as input loads at the nodal locations. The load applied at any step is distributed within the material because the

TABLE 1. Typical mass transport properties and environmental conditions

Degrees Orientation to Ply with Respect to Radial Axis	Material Number	Material Type	Diffusivity (cm^2/s)		Solubility (g/cm^3-atm)	Hygrothermal Coefficient (in./in. weight fraction of H_2O)
			D_R	D_Z	S	β
0, 15, 115	1-3	Graphite Phenolic	2.9×10^{-8}	2.3×10^{-8}	1.5	0.5
	4	Adhesive	1×10^{-9}	1×10^{-9}	2.18	0.5

Initial Conditions: equilibrated at 70°F/25 percent relative humidity
Boundary Conditions: constant at 70°F/70 percent relative humidity
Gap Opening: 0.001 in.

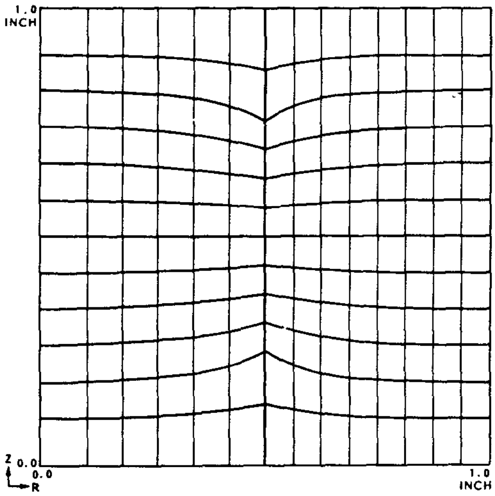


Fig. 5. Humidity analysis spatial mesh.

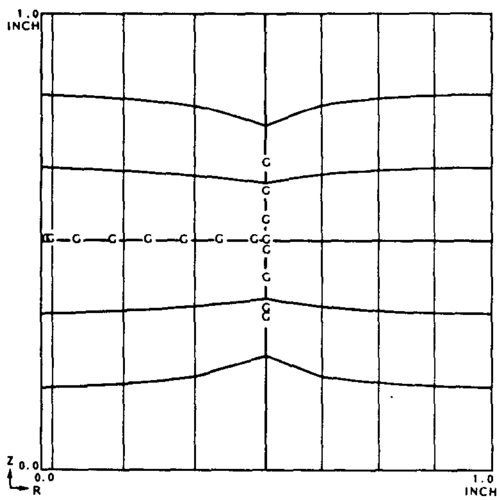


Fig. 6. Mechanical analysis spatial mesh; 'G' marks the location of gap elements.

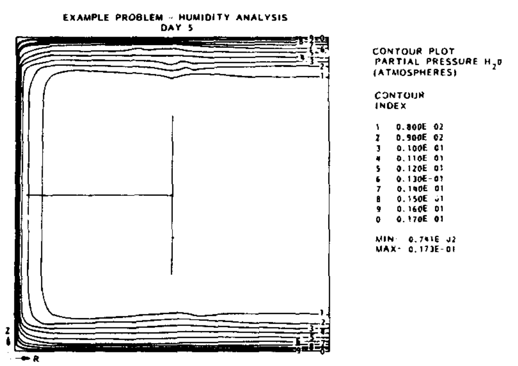


Fig. 7. Humidity analysis results, Day 5.

moisture is distributed within the material. The mechanical response, then, is to a distributed field of moisture content, and not a uniform load as would be the case when no moisture gradients exist. The ensuing mechanical response is therefore not spatially uniform.

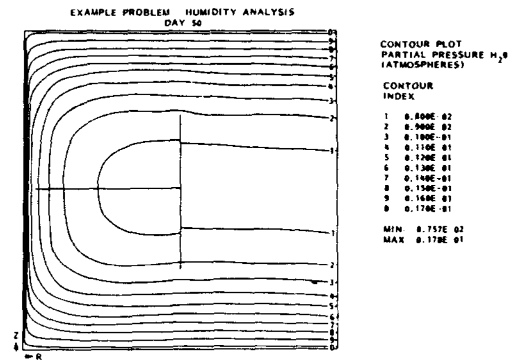


Fig. 8. Humidity analysis results, Day 50.

Radial and axial stress contours are plotted in Figs. 9 and 10. The internal stresses created result from the moisture absorption at day 50. The contours of stress roughly follow the contours of moisture content. A stress-free region exists at the center of the structure where no changes in the moisture concentration have yet occurred. The stress gradients also tend to concentrate at the adhesive bondlines, where the loads are transferred from material to material. In this example, the radial and axial stresses are primarily compressive. The moisture absorption tends to counteract any applied tensile loads at the bondline by virtue of the moisture induced compressive stresses.

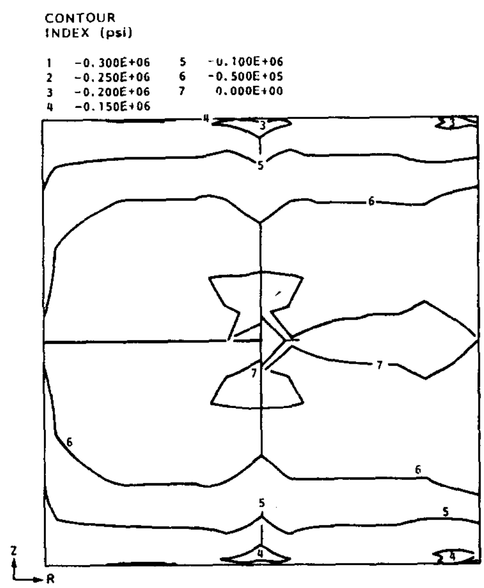


Fig. 9. Day 50, Radial stresses.

This example problem produced relatively low stresses in the region of gap closure at the left-most side of the composite assembly (Fig. 9). This is due to our choice of mechanical constraints in this example, which are remote from the gap. This lack of constraints near the location of gap closure allows sufficient degrees of freedom for swelling to occur to prevent the buildup of stresses.

The results given here are, of course, problem dependent and are meant to be illustrative of the computational methodology. Hence, the stresses and strains induced by the moisture

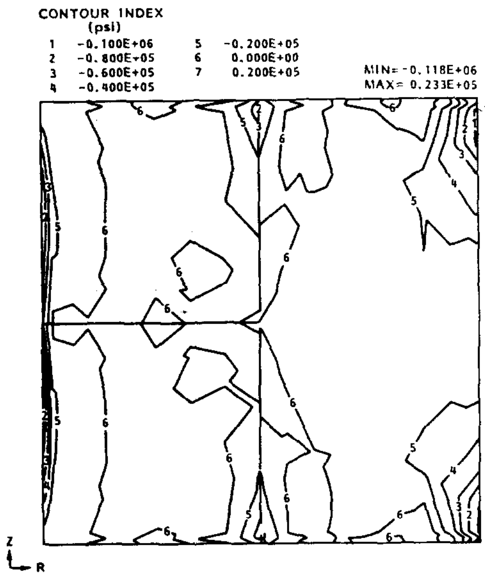


Fig. 10. Day 50, Axial stresses.

absorption in this example are not indicative of this phenomenon in general. It is conceivable that certain combinations of geometry, materials, environmental conditions, constraints, and applied loads could lead to resultant stress and strain fields quite different than illustrated here.

SUMMARY AND DISCUSSION

These results show that moisture penetration into a structure made of composite materials may be quite nonuniform when (1) the material properties governing moisture diffusion are orthotropic (or anisotropic) and (2) significant gaps or discontinuities in properties exist, separating one region from another. Further, the stress distributions produced by moisture diffusion into structures with nonuniform properties may be fairly complex, even when the structure geometry and loading conditions appear relatively simple. The results also suggest that gap closure (or opening) may be nonuniform when the moisture penetration and/or stress distribution is nonuniform. Therefore, computational modeling of the combined moisture diffusion and mechanical effects may be necessary to elucidate important structural responses to environmental factors.

ACKNOWLEDGEMENTS

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