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Two-Dimensional Hygrothermal Diffusions Into a Finite Width Composite Laminate

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ABSTRACT

Results are obtained for 2-D hygroscopic diffusion into composite laminates with free edges through the use of a second order finite difference scheme. A computer program was developed for the transient nonlinear coupled hygrothermal diffusion into finite width laminates with varying surface conditions along two edges. The formulation permits the diffusion coefficient to be a function of temperature, moisture concentration, and fiber orientation. The moisture distributions thus obtained are necessary for analysis of the moisture induced interlaminar stresses in the vicinity of free edges. It is shown that large diffusion times tend to eliminate the significance of stacking sequence, but gradients within and between layers are significant for all diffusion times.

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INTRODUCTION

Problems associated with combined thermal and mositure effects in polymeric matrix composite materials are currently receiving considerable attention on the part of the materials research community. The experimental works of McKague et al [1] and Browning et al [2,3] have shown that there is a degrading effect on the shear, compression and transverse stress properties of resinous composites due to moisture absorption. These degrading effects are primarily due to changes in properties of the resinous matrix and the fiber-matrix interface. McKague et al also presented rather extensive experimental results showing that the rate of moisture absorption is temperature dependent with the rate of absorption increasing with increasing temperature. It was also shown in reference [3] that large moisture concentration gradients may exist near the surfaces of composite laminates. These gradients may be significant because of the possibility of large interlaminar stresses near the free edge of composite laminates.

Analytical treatments of moisture diffusion in composites have been presented by several authors. Shen and Spring [4] considered one-dimensional absorption and desorption of homogeneous materials and composites, and Whitney [5] considered three-dimensional moisture diffusion in laminated composites. The emphasis in both of the above papers was on the total percent moisture weight gain as a function of time. Whitney also presented moisture profiles for two-dimensional diffusion into a laminate. These profiles were generated assumming the diffusion coefficient was an averaging of the laminates constituents. Since edge effects were included through a correction factor and were not treated explicitly in either of these two later papers, the significance of laminate stacking sequence wasn't readily assessable.

This paper presents numerical results for two-dimensional moisture diffussion into a symmetric finite width composite laminate. The results were obtained from a recently developed finite difference computer capability, denoted HYDIP, and the associated graphics program HYDIPG. This program was developed for the two-dimensional solution of the transient nonlinear coupled hygrothermal diffusion into a symmetric finite width composite laminate with varying surface conditions along two edges. The moisture distributions thus obtained are necessary for analysis of the interlaminar stresses which may be present in a composite laminate with free edges since these interlaminar stresses often initiate failure.

2. PROBLEM FORMULATION

The governing 3-D field equation for hygroscopic or thermal diffusion into a body is given by

$$\frac{\partial}{\partial x}\left(K_x \frac{\partial R}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial R}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial R}{\partial z}\right) = \frac{\partial R}{\partial t} \qquad (1)$$

where K_x, K_y and K_z represent the diffusion coefficients in the x, y and z directions, respectively, and R is the temperature or moisture concentration at a point in the body. Restricting the problem to that of a finite width symmetric laminate wih no variation in the x direction, figure (1), only a quarter laminate need be analyzed. The governing field equation becomes:

$$\frac{\partial}{\partial y}\left(K_y \frac{\partial R}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial R}{\partial z}\right) = \frac{\partial R}{\partial t} \qquad (2)$$

with symmetry boundary conditions

$$\left.\frac{\partial R}{\partial z}\right|_{z=0} = 0; \left.\frac{\partial R}{\partial y}\right|_{y=0} = 0 \tag{3}$$

and variable surface conditions

$$R = R(z)\big|_{y=b}; \; R = R(Y)\big|_{z=H}. \tag{4}$$

More specifically for the case of hygroscopic diffusion, the diffusion coefficient D may be a function of temperature T(y,z), moisture concentration M(y,z) and lamina fiber orientation θ,

$$D = D(T(y,z), M(y,z), \theta).$$

The governing field equations, (2) - (4), can now be written as

$$\frac{\partial D_y}{\partial y}\frac{\partial M}{\partial y} + D_y \frac{\partial^2 M}{\partial y^2} + \frac{\partial D_z}{\partial z}\frac{\partial M}{\partial z} + D_z \frac{\partial^2 M}{\partial z^2} = \frac{\partial M}{\partial t} \tag{5}$$

with symmetry boundary conditions

$$\left.\frac{\partial M}{\partial z}\right|_{z=0} = 0; \left.\frac{\partial M}{\partial y}\right|_{y=0} = 0 \tag{6}$$

and variable surface conditions

$$M = M(z)\big|_{y=b}; \; M = M(y)\big|_{z=H}. \tag{7}$$

3. SOLUTION SCHEME

The solution of the diffusion equation (5) was performed by a second order accurate variable step size finite difference scheme [6]. First and second derivative central difference derivatives are employed in the interior region of the laminate while only first derivative forward difference derivatives are necessary along the symmetry boundary conditions. A complete presentation of the basic difference equations used and the equivalent difference equation of equations (5) and (6) are presented in Appendix A.

Applying equations (A11) - (A13) at nodes throughout the laminate yields a set of linear simultaneous equations of the form

$$[C_t]\{M_{t+1}\} = \{P_t\} \tag{7}$$

where $[C_t]$ is the coefficient matrix at time t, $\{M_{t+1}\}$ are the unknown moisture concentration at time t+1 and $\{P_t\}$ is the right hand side vector which is a function of the moisture concentration at time t. It should be realized that at t = 0 $\{P_{t=0}\}$ would be a function of the initial moisture distribution. Equation (7) is then successively solved over N time increments. Transient problems can similarly be solved by imposing transient surface conditions in an incremental fashion.

An iterative simultaneous equation solution scheme [6], though more expensive to use for a single analysis, was chosen over an elimination or decomposition algorithm. This scheme was selected due to the incremental nature of the diffusion problem and because iterative schemes become cost efficient when successive solutions change only slightly from the previous results.

A Gauss-Siedel simultaneous equation solver was modified to efficiently solve equation (7) over N time intervals. This was primiarily achieved by eliminating the storage of zero coefficients and the multiplication by zeros. The required storage locations and multiplications of the modified Gauss-Siedel routine then become linear functions of the number of unknowns. A more detailed discussion of this solution scheme is presented in Appendix B.

4. CASE STUDIES

As mentioned in the introduction, large gradients in mositure concentration may exist near the free surfaces of a laminate. In this study it will be assumed that these gradients are the result of the laminate surface being subjected to an environment different from the one associated with the moisture distribution initially existing in the laminate. This condition could similarily be induced by thermal gradients in the composite as well as a variety of combinations of thermal and mositure distributions.

The initial studies investigated the effect of stacking sequence on the moisture distribution within the boundary layer region, approximately two lamina thicknesses along the laminates free edge. Material diffusion coefficients, [2], used in this study are shown in figure (2) while the laminates investigated are: $[90_2,0_2]_s$, $[90,0_3]_s$, $[0,90_2,0]_s$, $[90,0_2,90]_s$, $[0_2,90_2]_s$, $[0,\pm45,90]_s$, $[90,\pm45,0]_s$.

Upon examination of the laminates studied it becomes obvious that primarily $0_N/90_N$ combination laminates were considered. These laminates were chosen because they produce the most dramatic results due to the relative magnitude of the diffusion coefficients. Though the studies were very selective, the program HYDIP will handle any number of layers each at different fiber orientation and each having different material properties.

The basic model was a four layer symmetric laminate with 510 nodes on the model. Each layer, 0.005 in. thick and 1.0 in. wide, contains four nodes through the thickness with an additional node on the upper surface and 30 linearly spaced nodes across the width, Figure (1). The laminate was assumed to be initially dry and at a temperature of 440°K.

This temperature was chosen because the diffusion coefficient was much larger than that at room temperature as seen in Figure (2). An applied surface condition corresponding to 100 percent relative humidity was uniformly distributed along both free surfaces.

The plotted results in figures (3-13) have uniformly spaced nodes and are plotted with a slightly distorted aspect ratio to more readily visualize pertinent trends. As previously mentioned these plots represent a region of approximately two lamina thicknesses from the free edge.

Moisture distribution isoclines are numbered on each plot. Isoclines labeled 6 represent fully saturated conditions while those labeled 1 represents moisture concentrations of $1/6^{th}$ the saturated values.

5. RESULTS AND CONCLUSIONS

The effect of stacking sequence is most noticable after a short interval, on the order of 2-3 minutes, in a region near the free edge, as shown in Figures (3, 5, 8). This phenomena was typical of all laminates studied but will be shown using selected laminates. Transverse diffusion (z direction) reduces or eliminates the effect of stacking sequence for diffusion times greater than five minutes. This was indicative of all studies performed, especially in the outer region (see Figures (4, 7, 9, 11, 13) of the lamiante, but to a lesser extent in the inner region.

Large transverse gradients in moisture concentrations occurred within the outer layers with significant "corner" and "longitudinal" gradients in the adjacent and center most layer in all laminates studied, (Figure 3-13). Moisture diffusion was more uniform, i.e., smaller irregularities, with laminates having lower diffusion rates in the outer most layer. This is readily seen by comparing the time history contours of the $[0,\pm45,90]_s$ and $[90,\pm45,0]_s$ laminates as shown in Figures (10-13).

In conclusion, the stacking sequence was significant for very small diffusion times and in a region near the free edge. However, large diffusion times tended to eliminate the significance of stacking sequence due to the high transverse diffusion rates and aspect ratio of the composite laminate. Moisture concentration gradients within and between layers were significant for all diffusion times. From these results it is expected that large moisture gradients could produce large interlaminar stresses and greatly effect free edge delamination.

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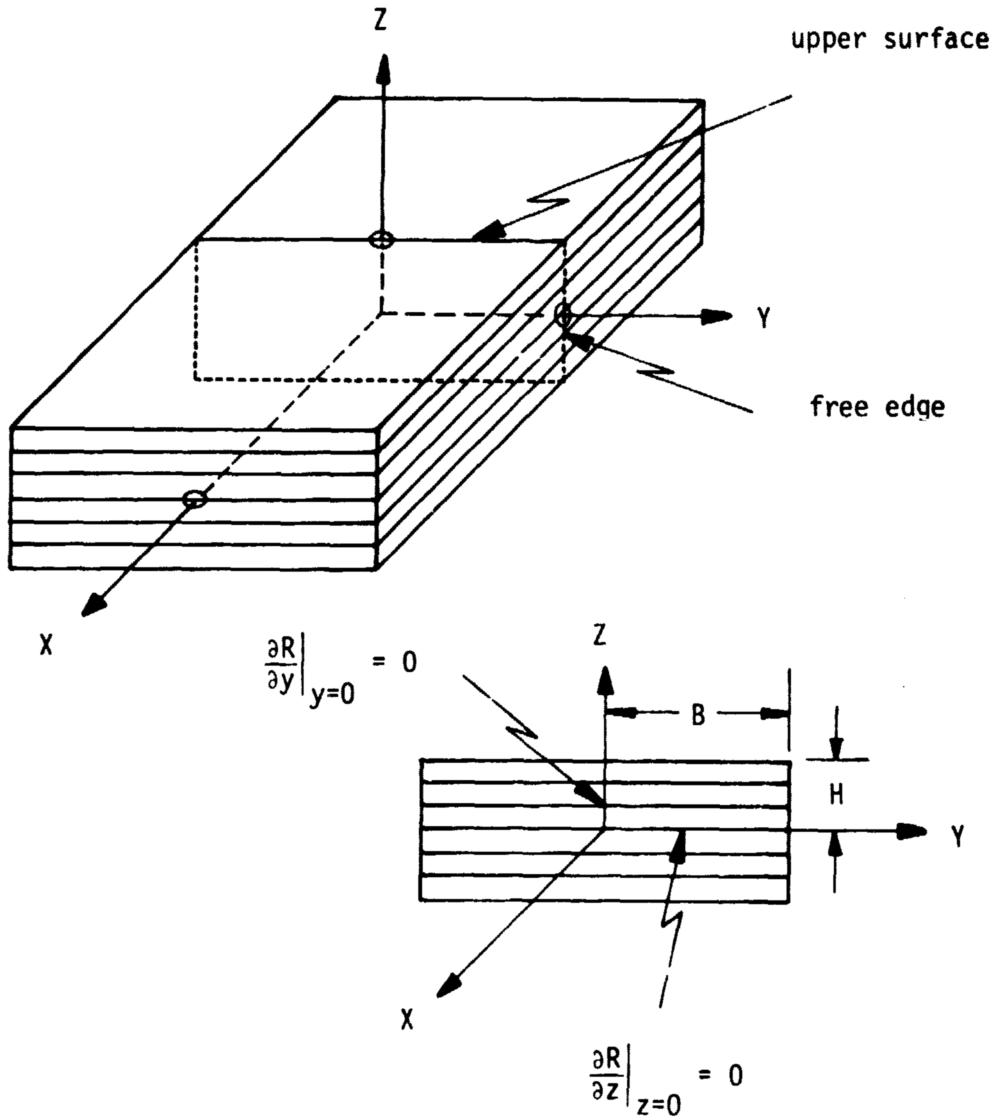

Figure (1) Symmetric Laminate with Boundary Conditions

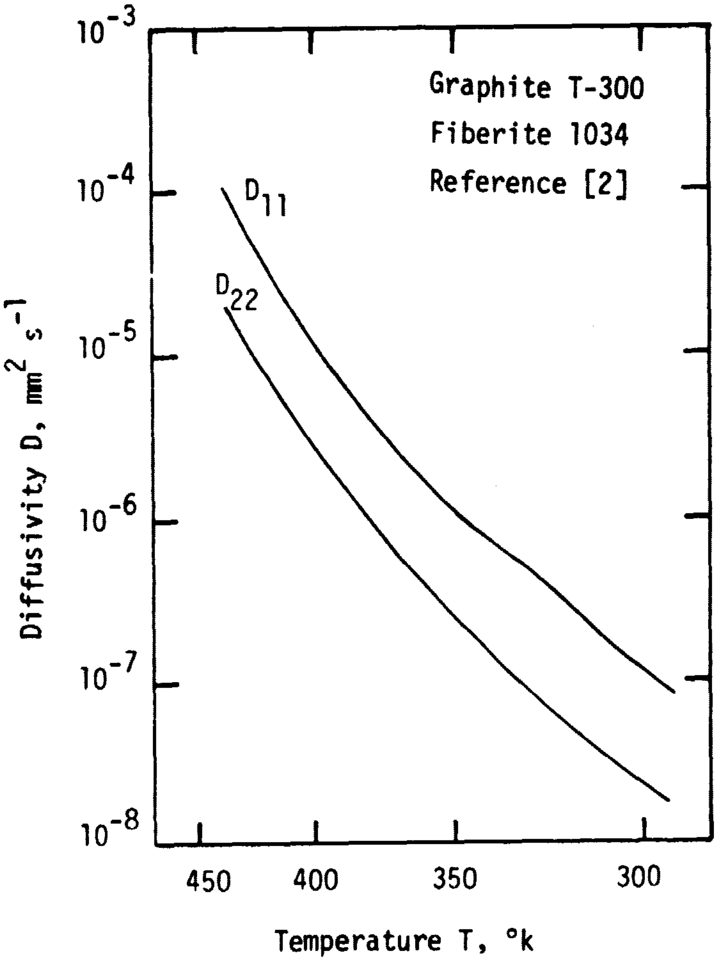

Figure (2) Longitudinal and Transverse Diffusion Coefficients vs. Temperature (°k)

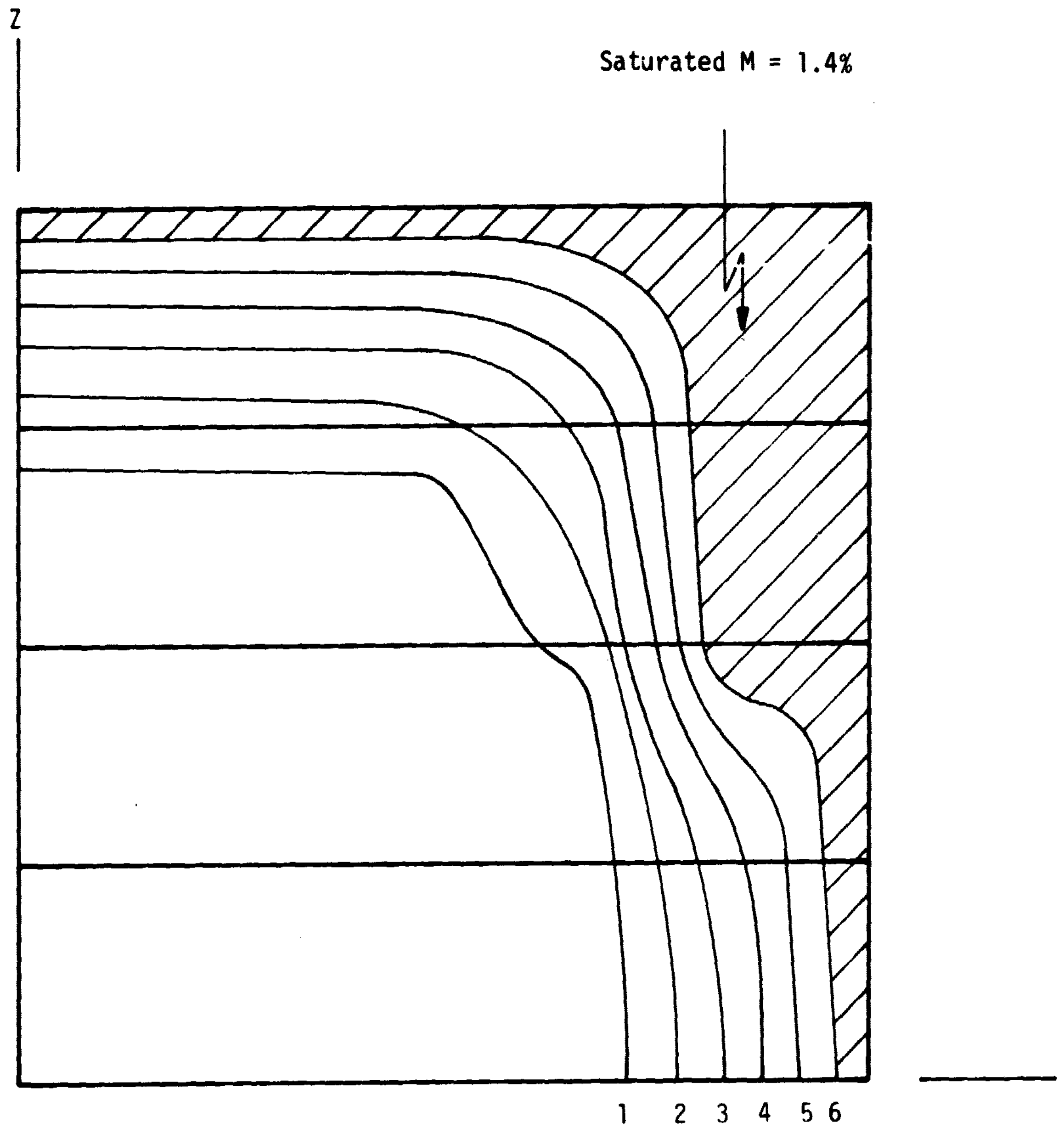

Figure (3) Moisture Concentration Contours in a $[90_2,0_2]_s$ Laminate at t = 150 sec.

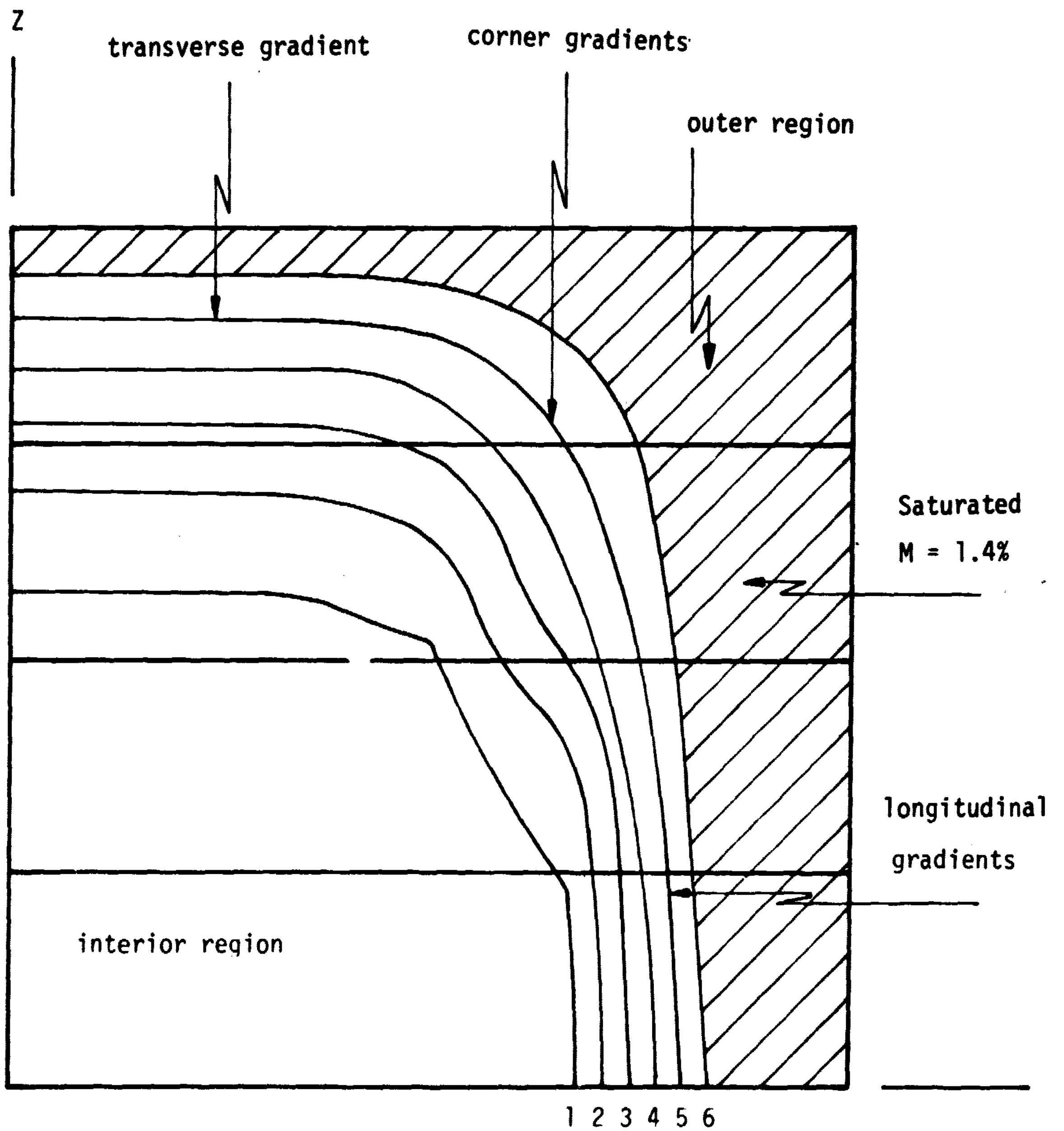

Figure (4) Moisture Concentration Contours in a $[90_2/0_2]_s$ Laminate at t = 300 sec.

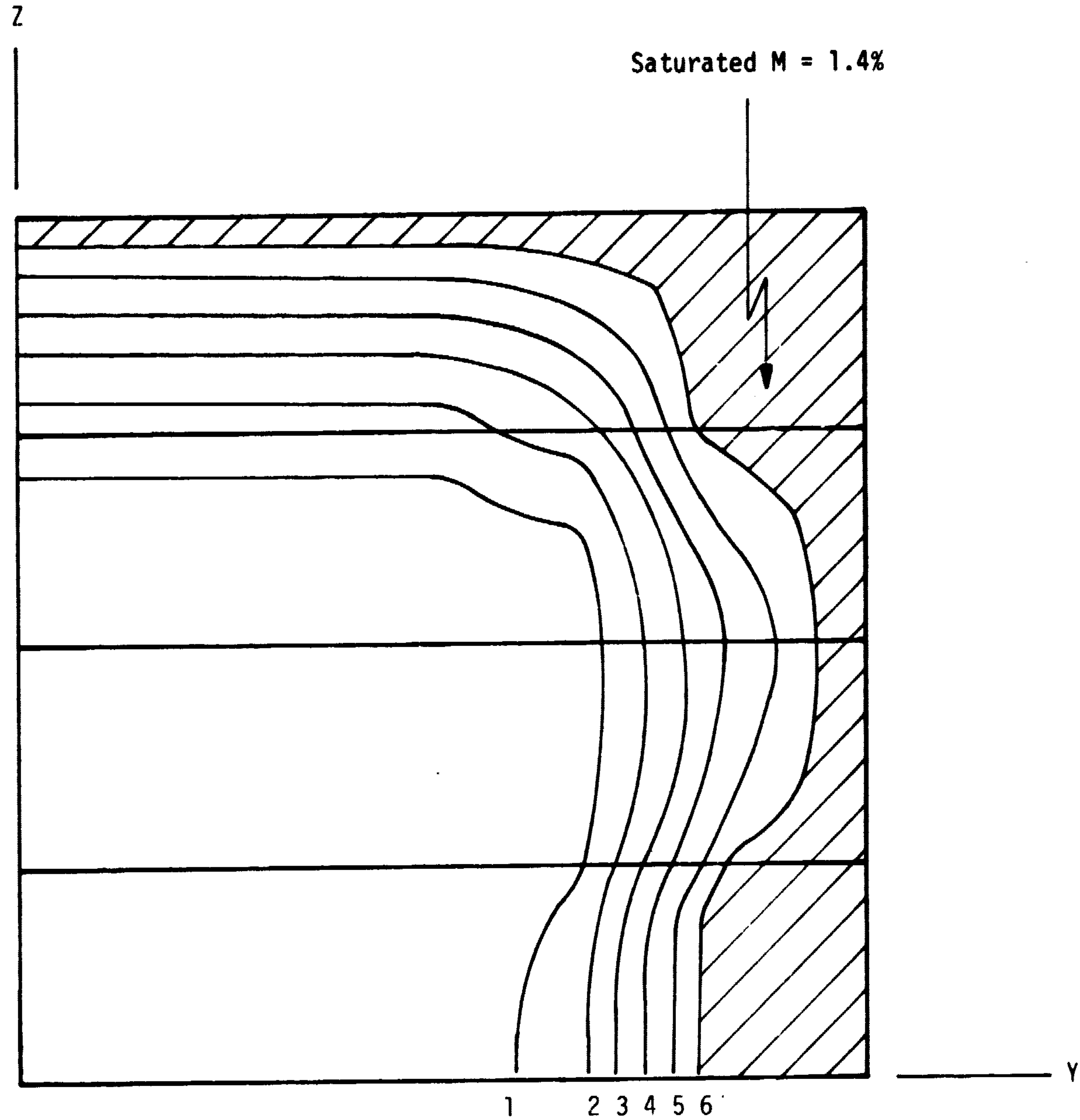

Figure (5) Moisture Concentration Contours in a $[90,0_2,90]_s$ Laminate at t = 150 sec.

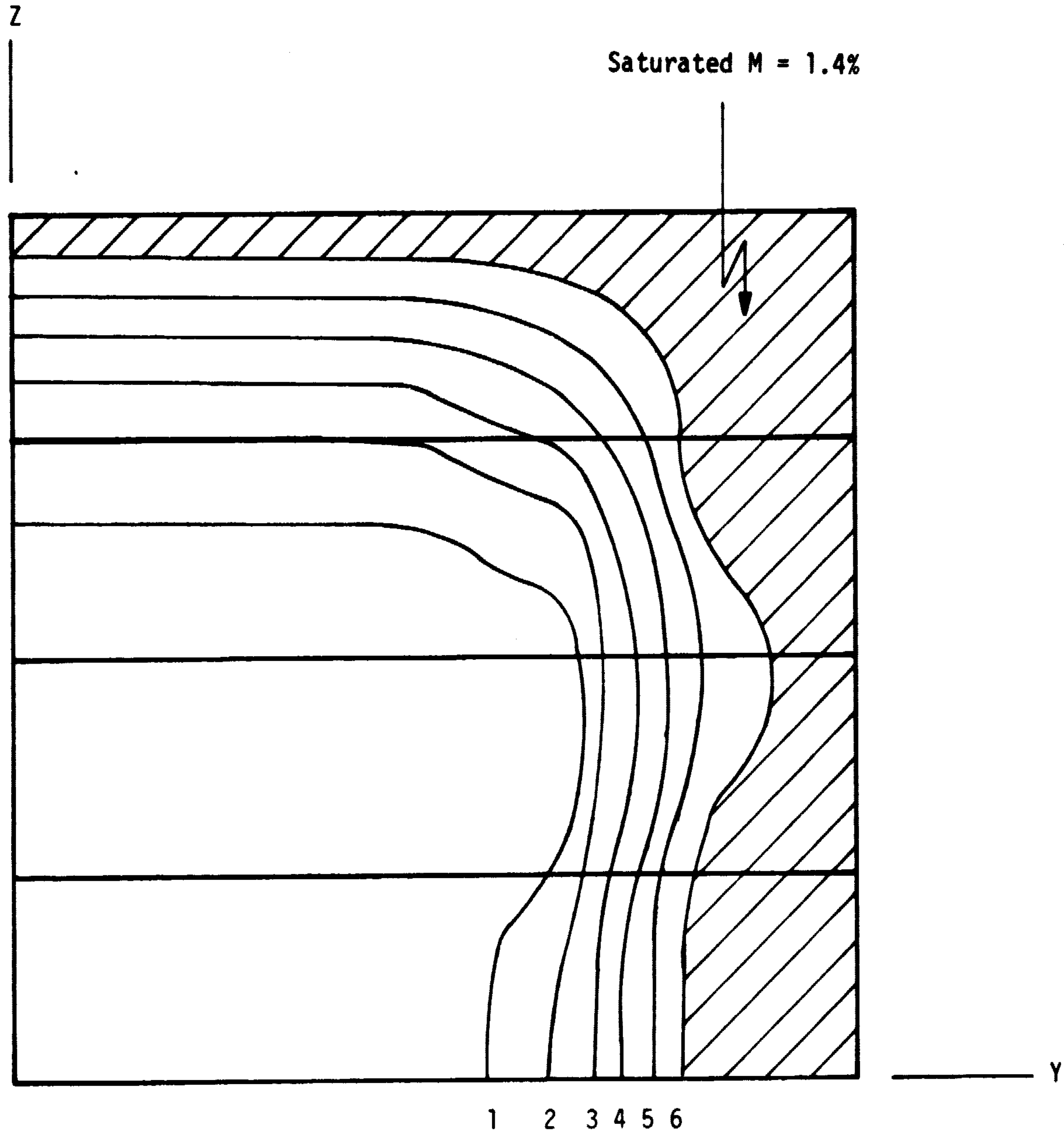

Figure (6) Moisture Concentration Contours in a $[90,0_2,90]_s$ Laminate at t = 200 sec.

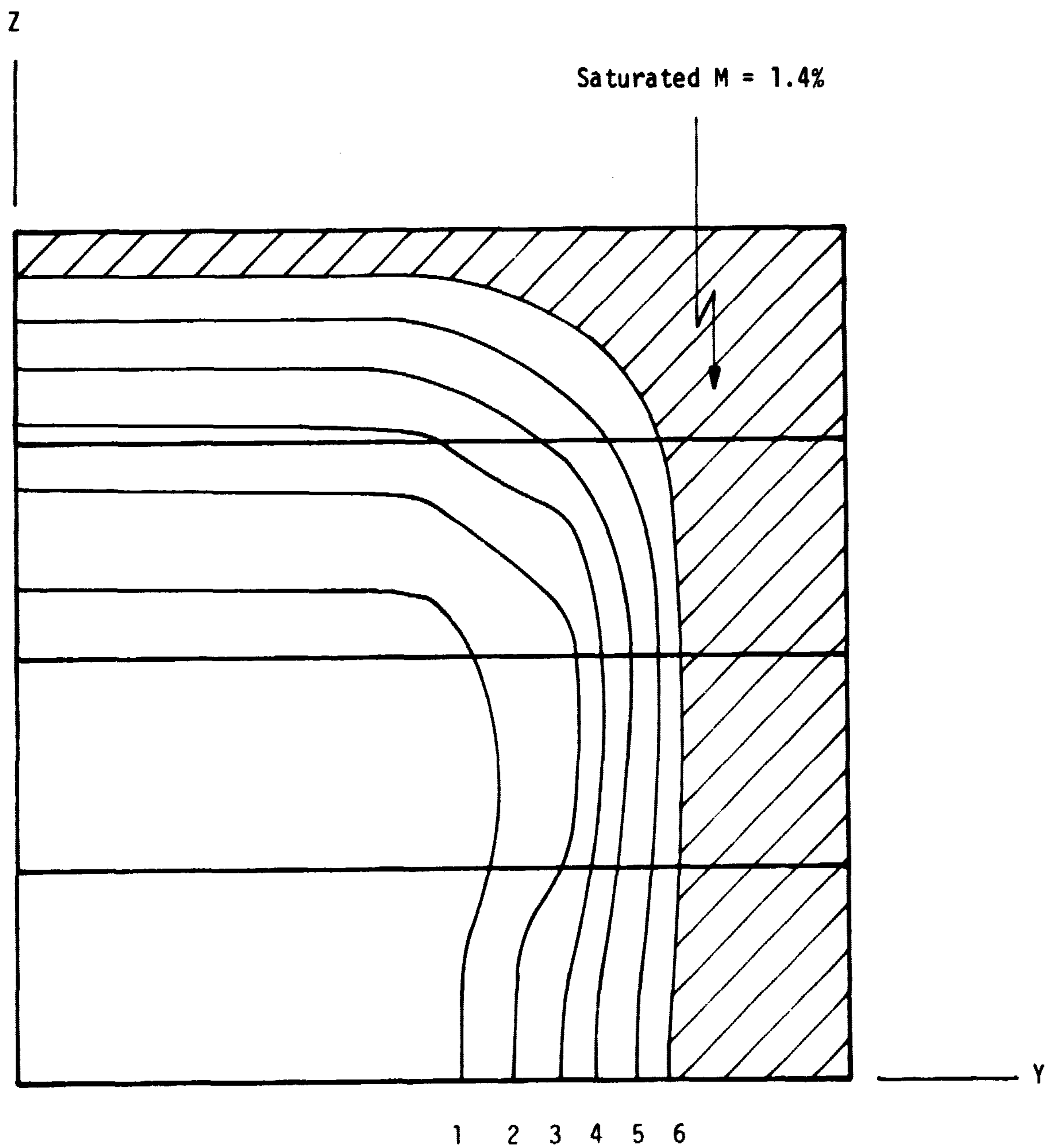

Figure (7) Moisture Concentration Contours in a $[90,0_2,90]_s$ Laminate at t = 300 sec.

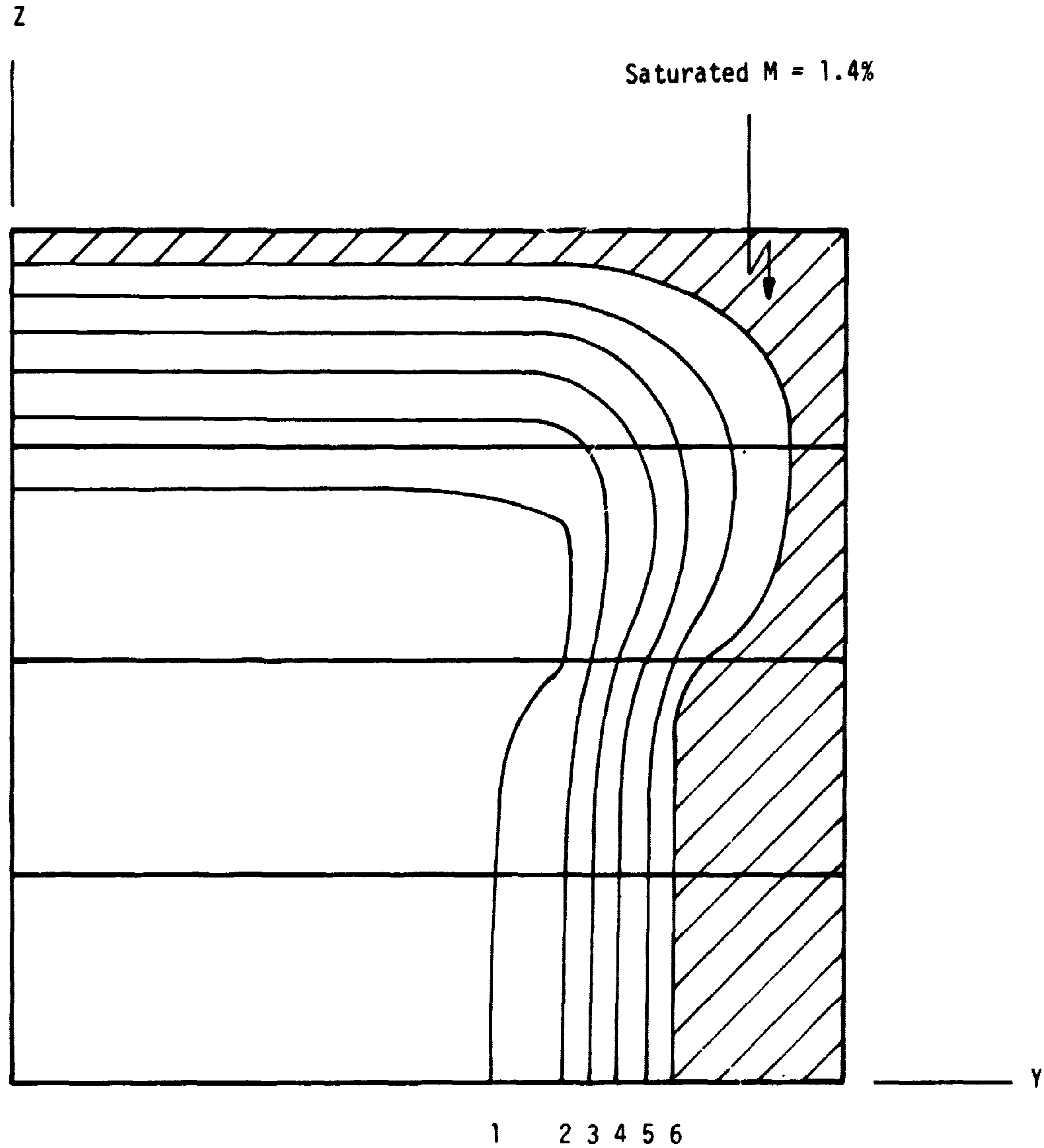

Figure (8) Moisture Concentration Contours in a $[0_2,90_2]_s$ Laminate at t = 150 sec.

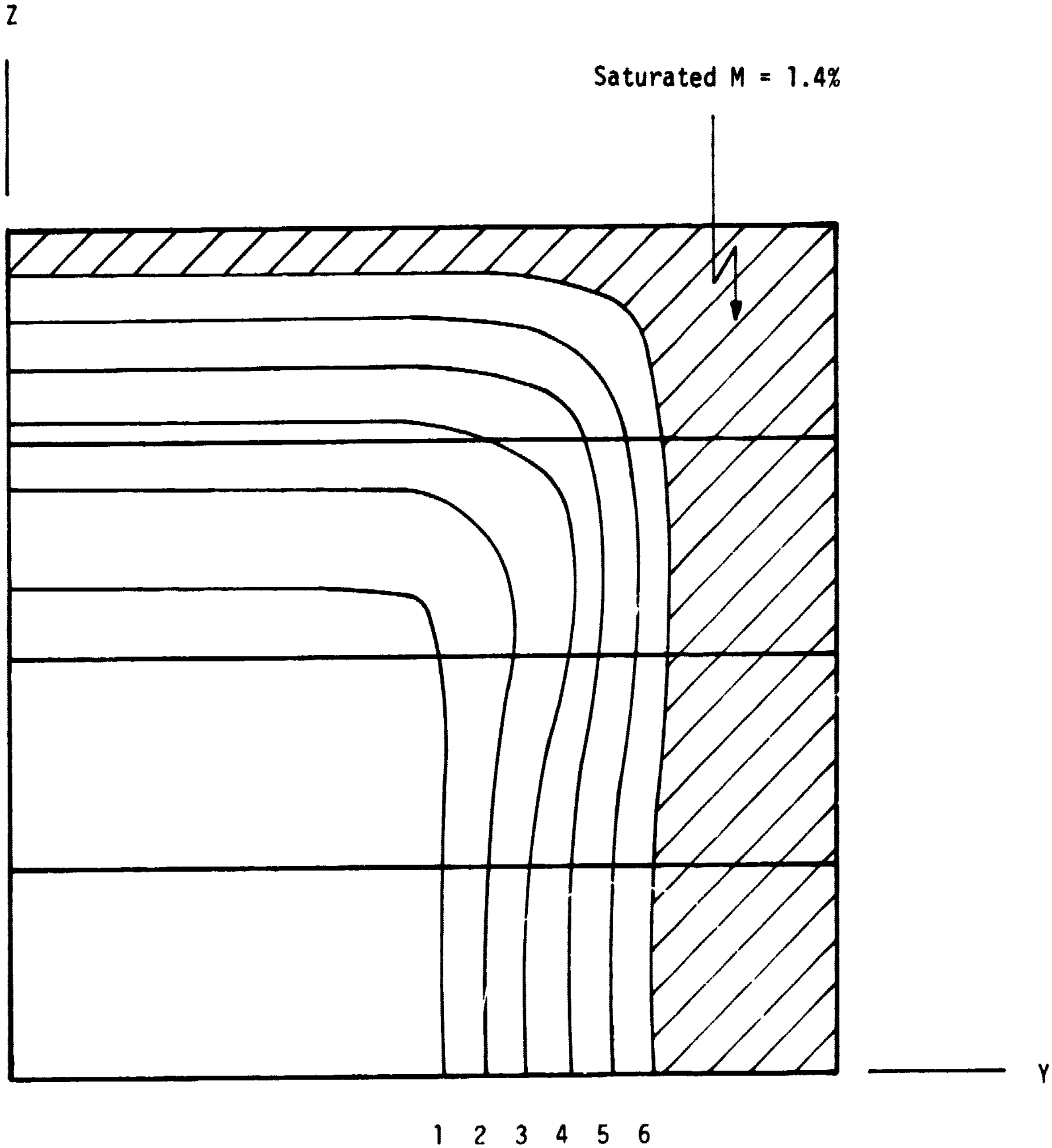

Figure (9) Moisture Concentration Contours in a $[0_2, 90_2]_s$ Laminate at t = 300 sec.

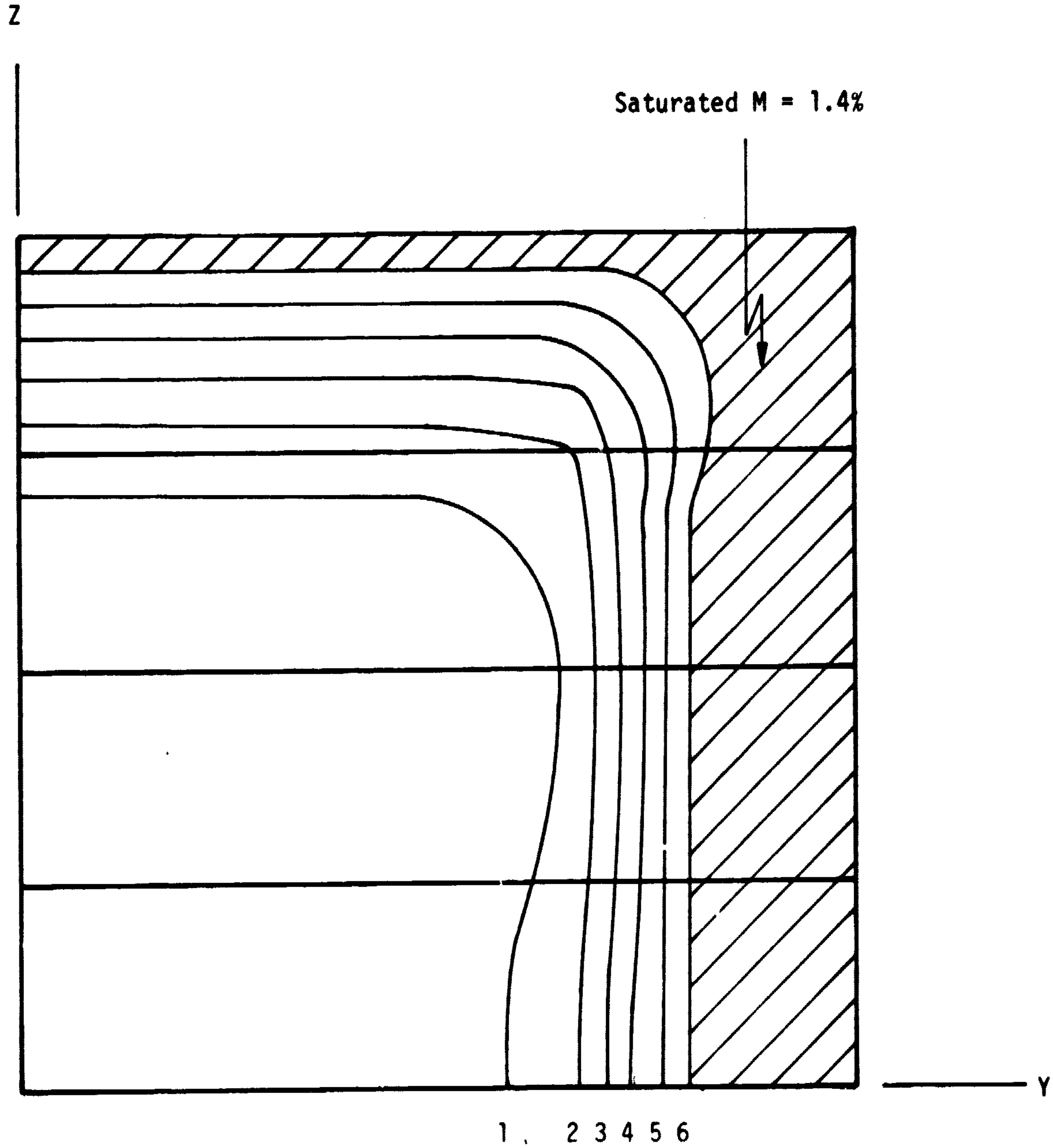

Figure (10) Moisture Concentration Contours in a $[0,\pm45,90]_s$ Laminate at t = 150 sec.

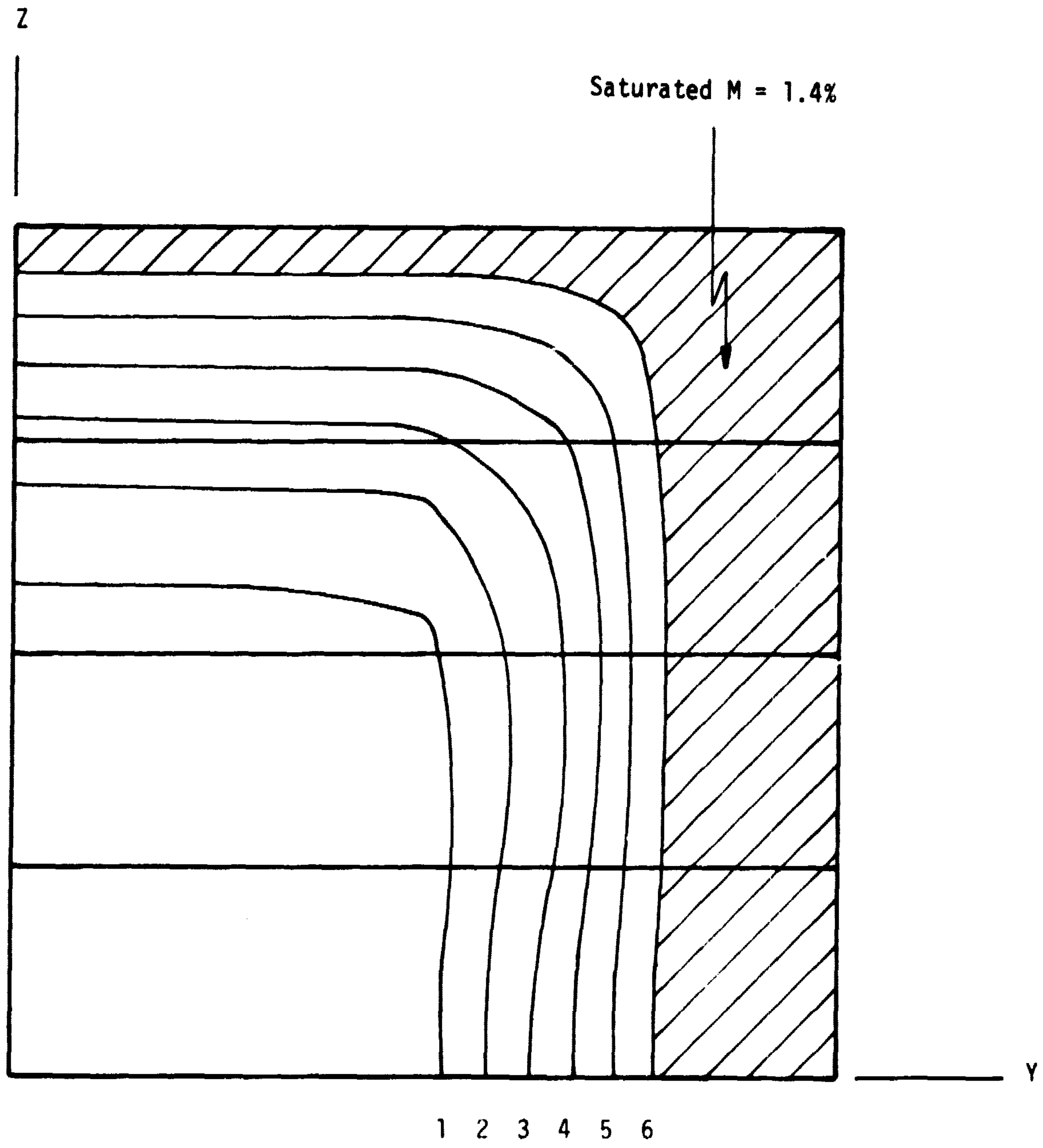

Figure (11) Moisture Concentration Contours in a $[0,\pm45,90]_s$ laminate at t = 300 sec.

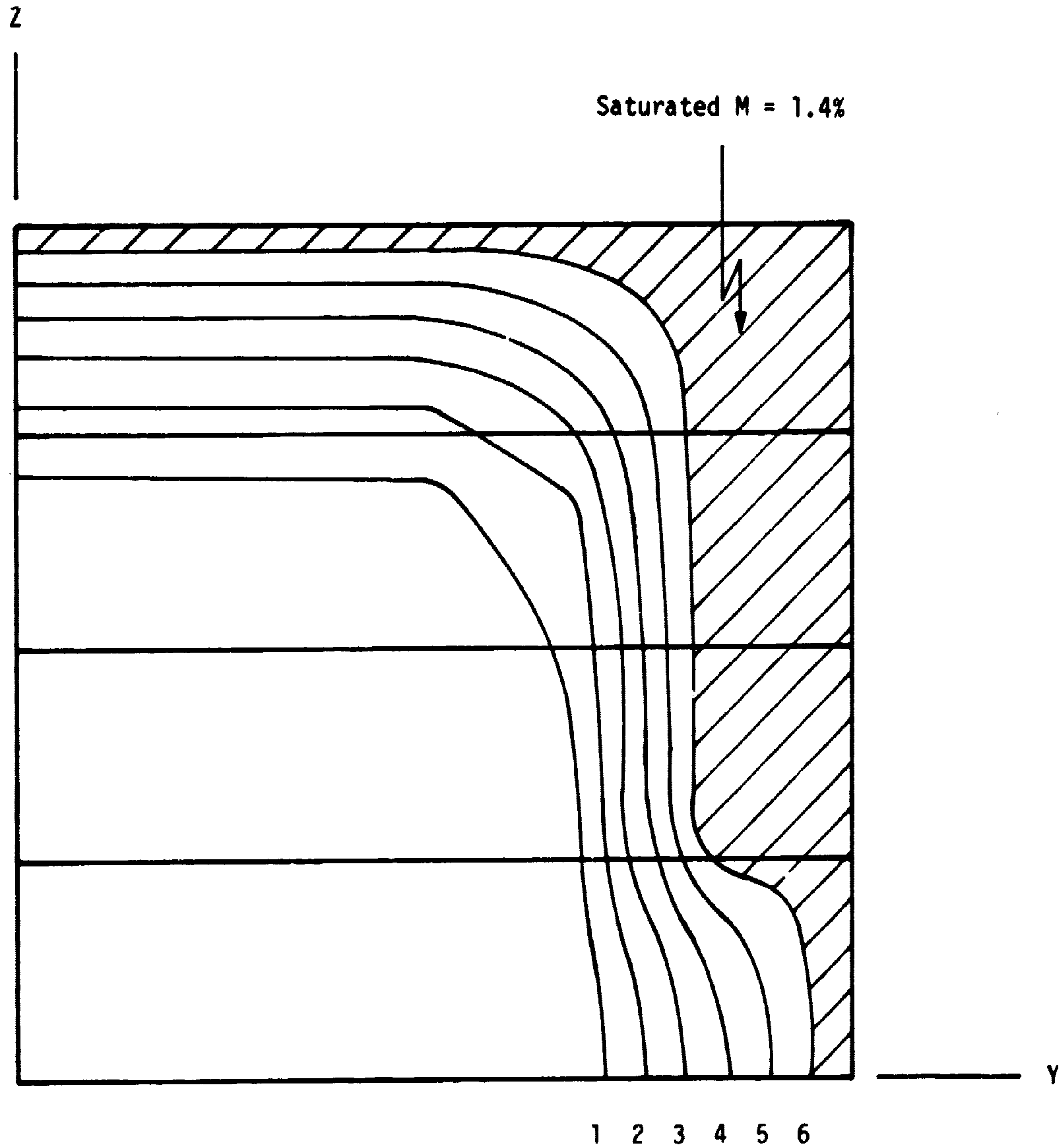

Figure (12) Moisture Concentration Contours in a $[90,\pm450]_s$ Laminate at t = 150 sec.

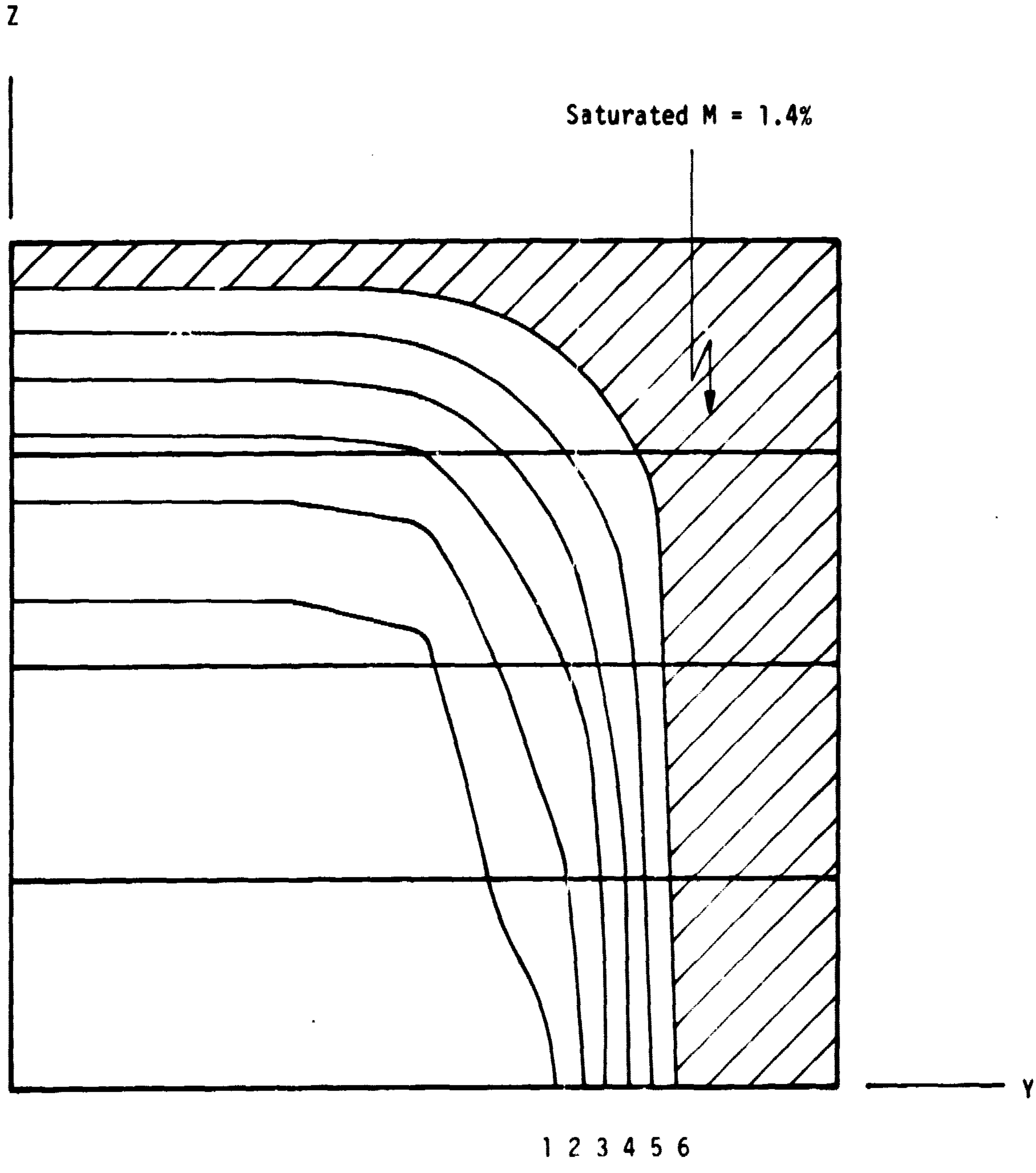

Figure (13) Moisture Concentration Contours in a $[90,\pm45,0]_s$ Laminate at t = 300 sec.

APPENDIX A

The finite difference derivatives were developed from a second order polynomial with unequal nodal spacing. The coefficients of the second order polynomial, (A1),

$$y = a_2x^2 + a_1x + a_0 \tag{A1}$$

can be determined by knowing the magnitude of y at three discrete points, x_0, x_1, x_2. Substituting these values of x and y into the polynomial, the a_i's can be determined through the matrix equation (A2).

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & h & h^2 \\ 1 & h(1+\alpha) & h^2(1+\alpha)^2 \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} y_0 \\ y_1 \\ y_2 \end{Bmatrix} \tag{A2}$$

where

$$h \equiv x_1 - x_0$$

$$\alpha \equiv (x_2 - x_1)/(x_1 - x_0)$$

The first derivative at $x = x_0$ in terms of h, α, y_0, y_1, and y_2 is;

$$D(y_0) = -\frac{y_0(\alpha+2)}{h(1+\alpha)} + \frac{y_1(1+\alpha)}{h\alpha} - \frac{y_2}{h\alpha(1+\alpha)} \tag{A3}$$

In a similar fashion the first and second central difference derivatives are;

$$D(y_0) = \frac{1}{h}\left[-\frac{\alpha y_{-1}}{(1+\alpha)} + -\frac{(1-\alpha)y_0}{\alpha} + \frac{y_1}{\alpha(1+\alpha)}\right] \tag{A4}$$

$$D^2(y_0) = \frac{2}{h^2}\left[\frac{y_{-1}}{(1+\alpha)} - \frac{y_0}{\alpha} + \frac{y_1}{\alpha(1+\alpha)}\right] \tag{A5}$$

Substituting equations (A4) and (A5) into (5) yields;

$$\frac{1}{h^2_{i,j}}\left[\frac{-\alpha_{i,j}\, D_{y_{i-1,j,t}}}{(1+\alpha_{i,j})} + \frac{(1-\alpha_{i,j})}{\alpha_{i,j}} D_{y_{i,j,t}} + \frac{D_{y_{i+1,j,t}}}{\alpha_{i,j}(1+\alpha_{i,j})}\right]$$

$$*\left[\frac{-\alpha_{i,j}\, M_{i-1,j,t+1}}{(1+\alpha_{i,j})} + \frac{(1-\alpha_{i,j})}{\alpha_{i,j}} M_{i,j,t+1} + \frac{M_{i+1,j,t+1}}{\alpha_{i,j}(1+\alpha_{i,j})}\right]$$

$$+ \frac{1}{k^2_{i,j}}\left[\frac{-\beta_{i,j}\, D_{z_{i,j-1,t}}}{(1+\beta_{i,j})} + \frac{(1-\beta_{i,j})\, D_{z_{i,j,t}}}{\beta_{i,j}} + \frac{D_{z_{i,j+1,t}}}{\beta_{i,j}(1+\beta_{i,j})}\right]$$

$$*\left[\frac{-\beta_{i,j}\, M_{i,j-1,t+1}}{(1+\beta_{i,j})} + \frac{(1-\beta_{i,j})}{\beta_{i,j}} M_{i,j,t+1} + \frac{M_{i,j+1,t+1}}{\beta_{i,j}(1+\beta_{i,j})}\right]$$

$$+ D_{y_{i,j,t}} * \frac{2}{h^2_{i,j}}\left[\frac{M_{i-1,j,t+1}}{(1+\alpha_{i,j})} - \frac{M_{i,j,t+1}}{\alpha_{i,j}} + \frac{M_{i+1,j,t+1}}{\alpha_{i,j}(1+\alpha_{i,j})}\right]$$

$$+ D_{z_{i,j,t}} * \frac{2}{k^2_{i,j}}\left[\frac{M_{i,j-1,t+1}}{(1+\beta_{i,j})} - \frac{M_{i,j,t+1}}{\beta_{i,j}} + \frac{M_{i,j+1,t+1}}{\beta_{i,j}(1+\beta_{i,j})}\right]$$

$$= \frac{1}{2\tau}\left[M_{i,j,t+1} - M_{i,j,t}\right] \tag{A6}$$

with boundary conditions obtained by substituting equation (A3) into (4). This yields;

$$\frac{-M_{1,j}(\beta_{1,j} + 2)}{(1+\beta_{1,j})} + \frac{M_{2,j}(1+\beta_{1,j})}{\beta_{1,j}} - \frac{M_{3,j}}{\beta_{1,j}(1+\beta_{1,j})} = 0 \tag{A7}$$

along z = 0 where i = 1, and

$$\frac{-M_{i,1}(\alpha_{i,1} + 2)}{(1 + \alpha_{i,1})} + M_{i,2} \frac{(1 + \alpha_{i,1})}{\alpha_{i,1}} - \frac{M_{i,3}}{\alpha_{i,1}(1 + \alpha_{i,i})} = 0 \qquad \text{(A8)}$$

along y = 0 where j = 1.

The coefficients used in equations (A6) - (A8) are defined as;

$M_{i,j}$ ≡ moisture concentration at the i,j^{th} node.

$h_{i,j}$ ≡ horizontal step size, (in the y direction)

$k_{i,j}$ ≡ vertical step size, (in the z direction)

$D_{y_{i,j,t}}$ ≡ diffusion coefficient in the y direction at node i,j determined from moisture and temperature data at time t.

$$D_{y_{i,j,t}} = D(T,M,Y,Z,\theta) = D_{22} \cos^2 \theta + D_{11} \sin^2 \theta.$$

D_{11}, D_{22} ≡ longitudinal and transverse differsion constants relative to the principal material coordinates.

$D_{z_{i,j,t}}$ ≡ diffusion constant in the z direction at the i,j^{th} node determined from moisture and temperature data at time t. In general $D_z = D_{22}$.

$\alpha_{i,j}$ ≡ ratio of distance between i-1, j-i and i, j-i+1, j nodes.

$\beta_{i,j}$ ≡ ratio of distance between i, y-1-i, j and i, j-i, j+1 nodes.

τ ≡ time increment

APPENDIX B

The unmodified Gauss Siedel simultaneous equation algorithm to solve equation (7) is of the form

$$\{M_{K+1}\} = \{D\} - [B]\{M_K\} \quad \text{(B1)}$$

where

$D_i = P_i/C_{i,i}$

$B_{i,j} = C_{i,j}/C_{i,i}$ for $i \neq j$

$B_{i,i} = 0$, with $i,j = 1,2,\ldots$ number of unknowns (NNUM)

and $\{M_K\}$ is continuously updated from the computed results of $\{M_{K+1}\}$.

This algorithm, as posed, requires storage on the order of $(\text{NNUM})^2$ and multiplications equal to $(\text{NNUM})^3$, per convergence iteration. Upon formulating the diffusion problem in conjunction with the Gauss Siedel solution scheme there are, at most, four non-zero $B_{i,j}$ coefficients per row. The number of non-zero coefficients is a function of the order of the difference equation and its order of accuracy. By eliminating the large number of zero coefficients in [B] and their multiplications the computer resources used to solve this problem would be greatly reduced. This was accomplished by developing only the non-zero [B] coefficients along with a series of pointer vectors relating them to the appropriate guess solution in vector $\{M_K\}$. As coded in HYDIP coefficient storage, including pointer vectors, is

9*(NNUM) locations while multiplications per convergence iteration equals 4*(NNUM).

Table (B1) presents a comparison of required computer resources to solve the diffusion problem using the modified Gauss Siedel, unmodified Gauss Siedel and a non-banded or blocked out of core Gaussian elimination algorithms. As seen from the table, the required computer resources varies linearly with respect to the number of unknowns for the modified Gauss Siedel algorithm while the other methods are quadratic or cubic functions of the number of unknowns.

Table B1. Storage and Computation Comparison of Three Solution Algorithms.

	Number of Unknowns	Number of Mult. and Divisions	Number of Storage Locations
Modified Gauss Siedel	100	400*	900
	500	2000*	4500
	1000	4000*	9000
Gauss Siedel	100	1×10^6*	10000
	500	1.25×10^8*	2.5×10^5
	1000	1.0×10^9*	1.0×10^6
Gaussian Elimination	100	2×10^5	10000
	500	1.42×10^6	2.5×10^5
	1000	8.9×10^7	1.0×10^6

* for the Gauss Siedel and the modified Gauss Siedel routines this represents the number of multiplications per convergence iteration.