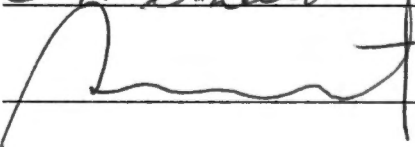


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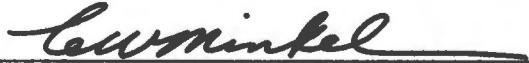
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Robert D. von Bernuth, Major Professor

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A THEORETICAL MODEL FOR MASS AND ENERGY CONSIDERATIONS
IN MICROCLIMATE MODIFICATION BY SPRINKLING

A Thesis
Presented for the
Master of Science
Degree
The University of Tennessee, Knoxville

Joel G. Hall
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ABSTRACT

Modification of the microclimate by irrigation sprinklers involves complex interactions among thermodynamic and transfer properties, system characteristics, and ambient conditions. A need exists for a better understanding of the theoretical background of these interactions. A theoretical model which accounts for the diffusion of heat and mass in stagnant air was developed for a two-dimensional radially axi-symmetric coordinate system. The governing equations were derived by application of equations for conservation of mass and energy. The finite element method using three-node linear triangular elements and linear interpolation functions was employed to obtain numerical solutions to the governing equations. Testing of the model was performed by comparing simulated results with proven analytical solutions as well as experimental data. An example of how the model can be adapted to a specific application is included for the case of heat and mass transfer from droplets in flight. Results showed that the model accurately simulates changes in both temperature and mass concentration of water vapor in stagnant air.

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CHAPTER I

INTRODUCTION

Background and Justification

The role of irrigation in modern agriculture has changed somewhat in recent years. Technology is now available for uses other than supplying water needs of plants. Notable examples include municipal/industrial wastewater distribution, chemical application, and microclimate modification. The latter may be subdivided into two categories--heat stress reduction and frost protection.

Modification of the microclimate (i.e., within the irrigated area) involves complex interactions among thermodynamic and transfer properties, ambient conditions, and system characteristics. The flight of a droplet emitted from a sprinkler nozzle is accompanied by transfer of heat and mass due to temperature and concentration gradients which exist between the water and the air. In addition, the droplet undergoes a phase change from liquid to vapor as evaporation occurs during flight. If the ambient conditions were hot and dry, the result would be a decrease in the temperature and an increase in the moisture content of the air. Frost protection, on the other hand, utilizes the heat released during the phase change from liquid to solid to prevent the surface of a plant from freezing. System characteristics such as application rate and speed of rotation are also important. In both

cases, the simultaneous diffusion of heat and mass occurs between the water and the air.

Although much research has been conducted relating to specific results of these processes, a surprisingly small amount of effort has been directed toward the underlying theory. A better understanding of the simultaneous diffusion of heat and mass would be valuable. A general atmospheric model which could be modified for specific applications would be a useful tool for purposes of design and analysis.

Review of Previous Work

Evaporation Losses

From the standpoint of application efficiency, evaporation of water during sprinkling represents a loss. For this reason much experimental work has been conducted in this area. Christiansen (1942) attempted to measure evaporation from the spray as the difference between the amount of water falling in an area and that which was discharged from the sprinkler. He used containers evenly spaced over an area to collect the water. These tests resulted in losses ranging from 10 to 42 percent for afternoon conditions in California. It was impossible, however, to separate evaporation losses which occurred from the spray and those which occurred from water clinging to the containers. Sunshine appeared to have a significant effect, while very little correlation was observed between evaporation and relative humidity or vapor pressure deficit.

Christiansen suggested an indirect method for estimating evaporation losses from the spray based upon the thermodynamic principles involved. Neglecting radiant heat, the following equation was presented:

$$E = \frac{100 \, c \Delta t}{r} \left[\frac{p_w - p_a}{p_w - p_a - 0.00037B(t_a - t_w)} \right] \quad (1-1)$$

where:

E = loss of water from the spray expressed as a percentage of total discharged

c = specific heat of water, cal/gm °F

r = heat of vaporization, cal/gm

Δt = temperature drop of the water from the time it leaves the nozzle until it reaches the ground, °F

t_w = mean water temperature, °F

t_a = air temperature, °F

p_w = pressure of the water vapor at t_w , inches Hg

p_a = pressure of the water vapor in the air, inches Hg, and

B = barometric pressure, inches Hg

The temperature drop of the water ranged from 1 to 20.7 °F, corresponding to a maximum loss of about 2 percent. Based on these results, Christiansen concluded that evaporation loss from the spray is negligible when compared to subsequent losses from the wet soil and vegetation.

Estimates of evaporation were made by Mather (1950), who observed the increase in moisture content of the air. Two types of irrigation systems were examined: overhead sprinkler lines and rotating sprinklers. For both cases, dewpoint readings were obtained along the windward and leeward direction relative to the sprinkler. The maximum increase in moisture content occurred downwind near the surface of the ground. This suggests that a large portion of the evaporation occurs from water on the ground or on the leaves of plants.

For an overhead sprinkler line Mather presented the following equation for evaporation as a percentage of the amount of water applied:

$$E = \frac{\rho u h (W_{up} - W_{dn})}{A l} \quad (1-2)$$

where:

W_{up}, W_{dn} = mean mixing ratios upwind (out of irrigated area) and downwind (within the irrigated area)

ρ = density of air, gm/cm³

h = vertical distance to homogeneous air, cm

u = wind velocity, cm/s

l = distance between upwind and downwind points, cm, and

A = depth of water applied, cm

Evaporation losses between 4 and 30 percent were observed in experiments using an overhead line. These figures represent losses from both the spray and the moist soil. Examination of the incremental evaporation

(i.e., the evaporation between successive observation points within the irrigated area) revealed losses ranging from 0 to 12 percent. Based on these data, Mather concluded that the evaporation decreased as the irrigated area increased.

Evaporation from a rotating sprinkler was found to be less than that from an overhead lateral. A slightly different equation was used for this case:

$$E = \frac{\rho u B (W_{\text{sat}} - W_o)}{A \pi r^2} \quad (1-3)$$

where:

$(W_{\text{sat}} - W_o)$ = change in mean mixing ratio between original air and saturated air

B = cross-sectional area under spray, cm^2

r = radius of the spray, cm

u = wind velocity, cm/s

ρ = density of the air, gm/cm^3 , and

A = depth of water applied, cm

Losses for the rotating sprinkler were on the order of 10 percent.

Frost and Schwalen (1955) developed a nomograph for estimating spray losses based on temperature, wind movement, operating pressure, humidity, nozzle size, and breakup of the spray. Losses as high as 45 percent were observed under extreme conditions of bright sunlight, high temperature, and low relative humidity. A high correlation

between evaporation and vapor pressure deficit of the atmosphere (the difference between the vapor pressure of the moisture in the air and the saturation vapor pressure at the same temperature) was also observed. Vapor pressure deficits ranging from 0.05 to 0.95 psi were recorded. Spray losses were also seen to increase with temperature, wind movement, operating pressure, and degree of breakup of the spray. Evaporation decreased with increases in relative humidity and nozzle size.

George (1957) measured the difference in salt concentration of water in the lateral and the water collected in containers to determine the evaporation loss from the spray. Losses ranging from 2 percent at a relative humidity of 48 percent and low wind speed to 15 percent at a relative humidity of 15 percent and high wind speed were reported. A high correlation between evaporation loss and relative humidity was observed, but vapor pressure deficit was not found to be significant. George observed that evaporation losses were greater in the vicinity of the sprinkler and near the extreme boundary of the wetted area than in the intermediate zone.

Droplets near the sprinkler are generally small with large surface area per unit volume. The greatest water-to-air ratio occurs at the outer edge of the wetted area, and these droplets have the longest travel time. This observation provides insight about the importance of the droplet size distribution of a sprinkler. If droplets were primarily small, evaporation and drift losses would be expected to be significant. On the other hand, if droplets were mostly large, these

losses may be less significant, however, the energy associated with larger droplets might cause runoff and erosion problems.

Kraus (1966) investigated water losses due to evaporation and wind drift from medium-sized, single nozzle sprinklers under various operating conditions. Based on conservation of mass, the following equation was presented:

$$V_{sp} = K \Sigma V_i + \frac{K \Sigma V_i (C_i - CI)}{CI} + V_{dr} \quad (1-4)$$

where:

V_{sp} = average volume of water discharged by one sprinkler, ft^3

V_i = average volume of water collected in can i , ft^3

V_{dr} = average volume of water drift, ft^3

C_i = sodium content of water in can i , ppm

CI = sodium content of water in the lateral, ppm, and

K = ratio between the area of the field represented by one can to its cross-sectional area

Results compared well with those of Frost and Schwalen (1961). Total losses ranged from 3.4 to 17.0 percent for saturation deficits of 0.125 and 0.673 inches of mercury (0.061 and 0.33 psi), respectively. Kraus concluded that evaporation losses are approximately proportional to the saturation deficit or relative humidity with no obvious effects due to radiation and wind.

Smith (1968) developed an analog simulation of evaporation from droplets in flight. He used trajectory equations considering momentum

change due to variations in both velocity and mass. He included an evaporation function expressed in terms of the rate of change of droplet diameter resulting from evaporation:

$$\frac{dD}{dt} = - \left(\frac{K}{2\pi D} \right) \Delta P \quad (1-5)$$

where:

D = instantaneous diameter

ΔP = ratio of vapor pressure gradient between the air and the droplet surface to the partial pressure of the air

K = the product of the prevailing temperature and the transfer coefficient at the instantaneous velocity

The model was used to predict the effects of imposed velocity and evaporation during flight upon initial and final diameter. The results were inconclusive due to experimental difficulties, however, droplet diameter was seen to decrease along the trajectory. This was most pronounced for small droplets which possess more surface area per unit volume than large droplets.

Seginer (1971) investigated the effects of geometric configurations of the irrigated area on water losses during sprinkling. His model was based upon comparison between two sets of conditions: the real one, and a standard one in which no evaporation or wind drift occurred. He then defined the losses as the relative differences between the standard and real conditions during a time period multiplied by the sampling area. Losses were categorized as evaporation

from the spray, evaporation from the ground, and wind drift. Seginer's results showed a high correlation between water losses and both incoming radiation and air temperature. Seginer concluded that spray losses are insignificant relative to drift losses.

Goering, Bode, and Genhardt (1973) incorporated the equations developed by previous researchers (Ranz and Marshall, 1952; Smith, 1970) into a model for spray droplet deceleration and evaporation. The results showed that evaporation of droplets in flight is inversely proportional to the diameter. This investigation was made for droplets up to 135 micrometers in diameter with corresponding Reynolds numbers up to 120.

Droplets of this size make up a very small percentage of the total volume of water emitted from typical irrigation sprinklers. Again, the importance of the droplet size distribution is stressed.

Kohl and Wright (1974) utilized psychrometric relationships to predict the temperature drop and vapor pressure increase due to evaporation during sprinkling. The temperature drop and corresponding vapor pressure increase were approximated by the following equations:

$$\Delta T = \frac{EQL_v \rho_w}{uh \rho_a c_p} \quad (1-6)$$

$$\Delta e = e_{w2} \left[\left(\frac{\frac{m_{v1} RH_1}{100} + \frac{EQ \rho_w}{uh}}{m_{v2}} \right) \right] - \frac{e_{w1} RH_1}{100} \quad (1-7)$$

where:

- ΔT = temperature drop, °C
- E = evaporation, percent of discharge
- Q = sprinkler discharge, l/s/m line
- l_v = latent heat of vaporization of water, cal/gm
- ρ_w = density of water, gm/cm³
- u = mean wind speed at 2 meters, m/s
- h = height, m
- ρ_a = density of air, gm/cm³
- c_p = heat capacity, cal/gm °C
- Δe = vapor pressure increase, mb
- e_{w1} = saturation vapor pressure at T_1 , mb
- e_{w2} = saturation vapor pressure at T_2 , mb
- RH_1 = relative humidity at T_1 , percent, and
- RH_2 = relative humidity at T_2 , percent

They assumed evaporation loss of 5 percent, 20 percent relative humidity, 30 °C air temperature, and sprinkler discharge of 0.032 l/s per meter of line. For these conditions, the maximum predicted temperature drop and corresponding vapor pressure increase were 1.0 °C and 0.6 mb, respectively. Actual measurements in the field compared closely with these predicted values.

Clark and Finley (1975) measured evaporation losses in the Southern Plains of Texas by subtracting the amount of water collected within the sprinkler pattern from the amount discharged. Losses were highly correlated with wind speed and vapor pressure deficit. For

low wind speeds (less than 4.5 m/s) the evaporation losses were generally less than 10 percent, and vapor pressure deficit was the controlling factor. Losses increased exponentially when the wind speed was between 4.5 and 8.5 m/s with losses ranging from 10 to 30 percent. An average value of 15 percent was determined to be descriptive of evaporation losses in the Southern Plains.

Nurnberger et al (1976) developed a mathematical model to predict the microclimate modification of air near the ground by evaporation of an ultra-fine mist. Their model was based on the diffusion equations for liquid water, water vapor, and heat. These equations may be written in the following general form:

$$u(z) \frac{\partial \phi}{\partial x} = \frac{\partial}{\partial z} \left[K(z) \frac{\partial \phi}{\partial z} \right] + \phi(z, x) \quad (1-8)$$

where:

$u(z)$ = wind speed in the direction of mean flow

ϕ = general diffusive property

$K(z)$ = turbulent diffusivity profile

x = direction along the mean wind, and

z = height

Based on simultaneous solutions of the three diffusion equations using the Patankar and Spalding control volume integral technique (Patankar and Spalding, 1968), an evaporative cooling rate of 2 °C per gram of water evaporated per cubic meter of air, and a maximum cooling of 20 °C was predicted. In field tests the maximum observed cooling was 14.6 °C.

Spurgeon, Thompson, and Gilley (1983) modified an equation developed by Yazar (1980) which predicts above canopy spray evaporation loss using the electrical conductivity method. This approach uses the fact that as evaporation occurs, the solute concentration increases, thereby increasing the electrical conductivity of the applied water. Evaporation losses may be estimated by the difference between the electrical conductivity of the water at the crop canopy and at the sprinkler. The resulting equation was written in terms of wind speed and vapor pressure deficit:

$$E = 0.389e^{0.191u} \text{ VPD}^{0.698} \quad (1-9)$$

where:

E = evaporation as a percentage of the total amount applied

u = wind speed, m/s

VPD = vapor pressure deficit, mb, and

e = base of the natural logarithm

Observed losses were generally less than 10 percent of the total water applied, although losses as high as 30 percent were observed for short periods of time.

A simulation model to estimate kinetic energy, evaporation, and wind drift was developed by Edling and Chowdhury (1984). They conducted a series of tests to determine the effect of variations in wind speed, air temperature, humidity, and nozzle height. Based on their model, evaporation losses varied proportionally with air temperature, wind

speed, and nozzle height. Evaporation was inversely proportional to droplet size.

Frost Protection

Most of the work discussed thus far represents empirical developments relating to evaporation losses during irrigation. A summary of the results from the pertinent articles reviewed is shown in Table 1. There is obviously some disagreement about the magnitude of losses as well as the factors which influence the process of evaporation during sprinkling. This serves as further justification for a better understanding of the theoretical nature of the problem.

The reduction in temperature due to evaporation of water during sprinkling may be utilized to relieve heat stress during hot dry periods. In winter months, however, frost causes damage to many orchards and vineyards. Ironically, the application of water to trees and vines during cold weather can serve to protect the plants from freezing. This is due to the fact that as water freezes, it releases heat. When liquid water at 0 °C is changed to ice at 0 °C, 80 calories of heat are released per gram (Solomon, 1984). This is known as the heat of fusion of water.

In general, the amount of frost protection provided depends upon the amount of water applied and the application rate. The frequency of wetting and the speed of rotation of the sprinklers is also important from the standpoint of optimization (Wheaton and Kidder, 1974). Early attempts were made to relate the application rate to the rate of

Table 1. Comparison of Evaporation Losses Reported by Various Researchers.

Investigation	Evaporation Loss (%)	Principal Factor(s) ^a
Christiansen (1942)	10 - 42	Radiation
Mather (1950)	4 - 30	-----
Frost and Schwalen (1955)	Up to 45	Vapor pressure deficit
George (1957)	2 - 15	Relative humidity
Kraus (1966)	3 - 17	Vapor pressure deficit; humidity
Seginer (1971)	<2	Radiation; air temperature
Kohl and Wright (1974)	5	-----
Clark and Finley (1975)	15	Wind; vapor pressure deficit
Spurgeon et al. (1983)	10 - 30	Wind; vapor pressure deficit

^aMeteorologic factors which were highly correlated with observed evaporation losses.

heat loss from the plant (Perry et al., 1982). Businger (1965) and Gerber and Harrison (1964) developed models to determine application rates for frost protection for given atmospheric conditions. Both of these models incorporated a heat balance which required that the application rate be sufficient to supply the heat of fusion necessary to maintain a constant temperature above the critical value. Barfield, Walton, and Lacey (1981) pointed out that the previous models did not account for the effects of relative humidity. They included this parameter by calculating the energy loss from an ice covered leaf. The resulting model required that the rate of application of latent energy replace the energy lost plus the water lost by evaporation. Barfield et al. concluded that the error made in ignoring the effects of humidity can be very large, and may result in an application rate which is too low.

The timely operation of a sprinkler system designed for frost protection is crucial. When the system is first turned on, a reduction in temperature occurs due to evaporative cooling. The magnitude of the drop depends on the relative humidity of the air (Wheaton and Kidder, 1974). For this reason, the system should be started before the air temperature reaches freezing. Once started, the system should not be turned off until the wet bulb temperature is at least 34 °F, or higher if the wind is blowing (Wheaton and Kidder, 1974). Data from the San Joaquin Valley indicate that a range of 2-8 °F of protection may be provided by sprinkling.

Research Objectives

The overall objective of this research was to gain a better understanding of the transfer processes which accompany the application of water by irrigation systems. Emphasis was placed on the development of underlying theory rather than the physical effects such that a sound basis for evaluation and design could be established. The specific objectives of this study were:

1. To develop theoretical equations which describe the simultaneous diffusion of heat and mass in stagnant air;
2. To develop a generalized computer program to predict the temperature and moisture response resulting from the simultaneous diffusion of heat and mass in stagnant air;
3. To verify the accuracy of the model by comparison with proven solutions and experimental data; and
4. To illustrate the use of the model for the specific application of droplets in flight.

CHAPTER II

DEVELOPMENT OF THE MODEL

Conceptual Approach

The ability to define a problem is limited by the ability to conceptualize it. Therefore development of a mathematical model for a physical system begins at the conceptual level. This requires a basic understanding of the nature of the problem to be modeled.

Modification of the microclimate during sprinkling involves complex interactions among many factors. Inclusion of every interaction in the initial stages of model development is not realistic. Therefore a tradeoff exists between factors which should be included and those which may be omitted. The primary objective of this research was to develop a generalized atmospheric model which accounts for the diffusion of heat and mass in stagnant air. A decision was made not to include the effects of wind in the initial model, however, it is hoped that the effects of wind can eventually be incorporated. Based on the stated objectives, the problem reduces to two processes: diffusion of mass and diffusion of energy. The effects of these two processes are changes in temperature and moisture content of the air. The approach was to derive the governing equations based on conservation laws. The resulting differential equations were then solved numerically and expressed in a form suitable for coding into a computer. Having done

this, the model was initiated by specifying some initial conditions and monitoring the time response of the air temperature and moisture content.

Mathematical Background

Derivation of Governing Equations

The ability to mathematically express and, subsequently, to interpret the equations which describe system behavior is paramount to the success of the model. Care should be taken in the selection of system boundaries and in the making of assumptions. Inclusion of non-essential components complicates the analysis, however, exclusion of essential factors may result in erroneous results.

The first step in deriving the governing equations was to define the system. The geometry chosen for this model was a two-dimensional radially axi-symmetric system. This coordinate system is composed of radial and vertical axes which are symmetric about the central axis. Figure 1 illustrates this geometry and the elemental volume used in the development of the governing equations. Conservation laws (in rate form) for mass and energy were applied to this control volume to derive the equations.

Conservation of mass. Consider the elemental volume shown in Figure 1 as a control volume. A mass balance (in rate form) yields the following terms:

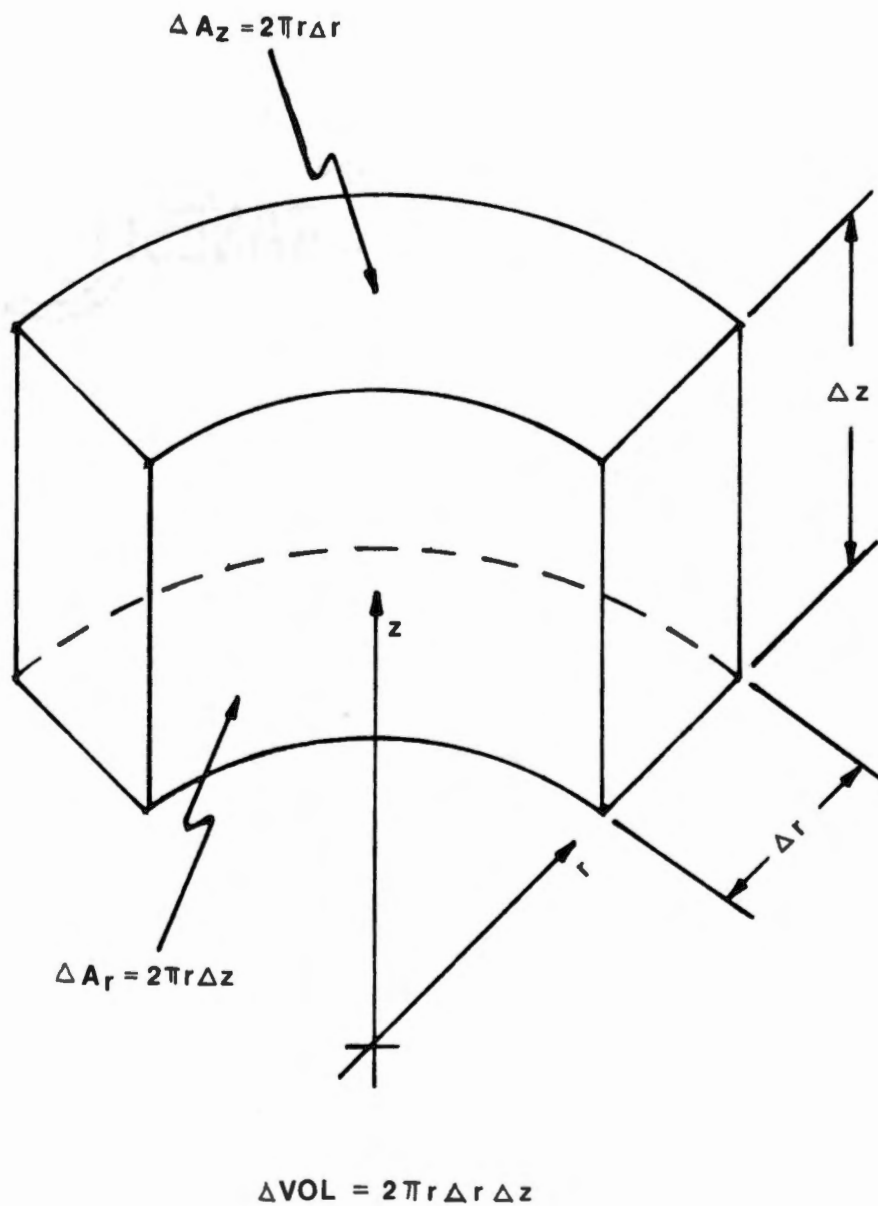


Figure 1. Geometry and Elemental Volume Used in Development of Governing Equations.

$$\dot{W}_{in} + \dot{W}_{gen} = \dot{W}_{out} + \dot{W}_{stor} \quad (2-1)$$

where:

$\dot{W}$ = rate of change of the mass of water vapor

$\dot{W}_{in}$ represents the rate of mass transfer into the system across system boundaries. Mass transfer may occur as a result of gradients in four quantities (Welty et al., 1976):

1. concentration
2. pressure
3. temperature (thermal diffusion or Soret Effect)
4. external forces

The effects of external forces, including gravity, were not considered in this analysis. Pressure was assumed to remain constant within the boundaries of the system, therefore this term was also neglected. The transfer of mass by temperature gradient (i.e., thermal diffusion) is important only when extreme temperature gradients are present (Grew and Ibbs, 1952). Since this condition was not expected in this study, thermal diffusion was assumed to be insignificant relative to diffusion due to concentration gradients. Based on these simplifications, $\dot{W}_{in}$ may then be written according to Fick's Law:

$$\dot{W}_{in} = - \left[DA_r \frac{\partial p_w}{\partial r} \right]_r - \left[DA_z \frac{\partial p_w}{\partial z} \right]_z \quad (2-2)$$

where:

ρ_w = mass concentration (mass density) of water vapor

D = diffusion coefficient

$A_r = 2\pi r \Delta z$

$A_z = 2\pi r \Delta r$, and

r, z = position coordinates for a radially axi-symmetric system

Similarly, $\dot{W}_{out}$, which represents the rate of mass transfer out of the system across system boundaries, may be expressed as follows:

$$\dot{W}_{out} = - \left[D A_r \frac{\partial \rho_w}{\partial r} \right]_{r+\Delta r} - \left[D A_z \frac{\partial \rho_w}{\partial z} \right]_{z+\Delta z} \quad (2-3)$$

The signs are negative in equations 2-2 and 2-3 because diffusion occurs in the direction of decreasing concentration (Crank, 1975).

$\dot{W}_{gen}$ represents the rate of mass generation within the system. Mass generation may be the result of chemical reactions or a change in phase such as evaporation within the volume. It is usually expressed as a rate per unit of volume:

$$\dot{W}_{gen} = V w''' \quad (2-4)$$

where:

w''' = rate of water vapor generation per unit volume

V = volume of the system ($2\pi r \Delta r \Delta z$)

In this form, the actual mechanisms of phase change are not explicitly being modeled. The generation term merely accounts for the specified value of mass generation assuming it to be in the form of water vapor. It would be possible to simulate the effects of a phase change by specifying the appropriate generation which satisfies the mass balance for the phase change. This allowed the model to be developed in a very general form while making provisions for specific applications.

$\dot{W}_{stor}$ is the rate of mass accumulated within the system boundaries. This term is a measure of the capacitance of the system and is a function of the system volume and time:

$$\dot{W}_{stor} = V \frac{\partial \rho_w}{\partial t} \quad (2-5)$$

where:

V = system volume, and

t = time

Substitution of equations 2-2 through 2-5 into 2-1 and rearranging terms gives the following expression:

$$V \frac{\partial \rho_w}{\partial t} - \left[DA_r \frac{\partial \rho_w}{\partial r} \right]_{r+\Delta r} - \left[DA_z \frac{\partial \rho_w}{\partial z} \right]_{z+\Delta z} + \left[DA_r \frac{\partial \rho_w}{\partial r} \right]_r + \left[DA_z \frac{\partial \rho_w}{\partial z} \right]_z - V w''' = 0 \quad (2-6)$$

If the actual expressions for A_r , A_z , and V are substituted into 2-6. the resulting equation is:

$$\begin{aligned} (2\pi r \Delta r \Delta z) \frac{\partial \rho_w}{\partial t} - \left[D(2\pi r \Delta z) \frac{\partial \rho_w}{\partial r} \right]_{r+\Delta r} - \left[D(2\pi r \Delta r) \frac{\partial \rho_w}{\partial z} \right]_{z+\Delta z} \\ + \left[D(2\pi r \Delta z) \frac{\partial \rho_w}{\partial r} \right]_r + \left[D(2\pi r \Delta r) \frac{\partial \rho_w}{\partial z} \right]_z - (2\pi r \Delta r \Delta z) w'''' = 0 \quad (2-7) \end{aligned}$$

The diffusion coefficient, D , is a function of pressure, temperature, and system composition (Welty et al., 1976). Since the pressure was assumed to remain constant, and the temperature range was assumed to be small, the diffusion coefficient was assumed to be constant.

Rearranging terms and dividing by $2\pi r \Delta r \Delta z$, equation 2-7 becomes:

$$\begin{aligned} r \frac{\partial \rho_w}{\partial t} - r w'''' - \left\{ \frac{D \left[r \frac{\partial \rho_w}{\partial r} \right]_{r+\Delta r} - D \left[r \frac{\partial \rho_w}{\partial r} \right]_r}{\Delta r} + \right. \\ \left. \frac{D \left[r \frac{\partial \rho_w}{\partial z} \right]_{z+\Delta z} - D \left[r \frac{\partial \rho_w}{\partial z} \right]_z}{\Delta z} \right\} = 0 \quad (2-8) \end{aligned}$$

Taking limits as Δr , Δz approach zero:

$$r \frac{\partial \rho_w}{\partial t} - r w'''' - D \frac{\partial}{\partial r} \left(r \frac{\partial \rho_w}{\partial r} \right) - D \frac{\partial}{\partial z} \left(r \frac{\partial \rho_w}{\partial z} \right) = 0 \quad (2-9)$$

Equation 2-9 is the equation for the conservation of mass for the system.

Conservation of energy. Development of the equation for conservation of energy followed the same procedure as that for conservation of mass. For the control volume shown in Figure 1, application of an energy balance yields the following terms:

$$\dot{E}_{in} + \dot{E}_{gen} = \dot{E}_{out} + \dot{E}_{stor} \quad (2-10)$$

Energy transfer may take several forms. The most common form is heat, which may occur by conduction, convection, and radiation (Carslaw and Jaeger, 1959). While the mechanisms of radiation and convection are potentially important effects, they were neglected at this stage of development. The only remaining mechanism for heat transfer is conduction. The driving force for conduction heat transfer is a temperature difference. Another factor which must be accounted for, however, is the change in internal energy which accompanies mass transfer into or out of the system. This effect is related to the enthalpy of the diffusing media. $\dot{E}_{in}$ may then be expressed as follows:

$$\dot{E}_{in} = q_{in} + h_w \dot{W}_{in} \quad (2-11)$$

where:

$$\begin{aligned} q_{in} &= -[KA_r \partial T / \partial r]_r - [KA_z \partial T / \partial z]_z \\ \dot{W}_{in} &= -[DA_r \partial \rho_w / \partial r]_r - [DA_z \partial \rho_w / \partial z]_z \quad (\text{from 2-2}) \\ h_w &= \text{enthalpy of the water vapor, and} \\ T &= \text{temperature of air-water vapor mixture} \end{aligned}$$

By substituting the equations for individual terms into 2-11, the rate of energy transfer into the system can be written as follows:

$$\begin{aligned} \dot{E}_{in} &= - \left[K(2\pi r \Delta z) \frac{\partial T}{\partial r} \right]_r - \left[K(2\pi r \Delta r) \frac{\partial T}{\partial z} \right]_z - \left[Dh_w(2\pi r \Delta z) \frac{\partial \rho_w}{\partial r} \right]_r \\ &\quad - \left[Dh_w(2\pi r \Delta r) \frac{\partial \rho_w}{\partial z} \right]_z \end{aligned} \quad (2-12)$$

Similarly, $\dot{E}_{out}$, the rate of energy transfer out of the system across system boundaries, may be expressed as shown below:

$$\dot{E}_{out} = q_{out} + h_w \dot{W}_{out} \quad (2-13)$$

where:

$$\begin{aligned} q_{out} &= -[KA_r \partial T / \partial r]_{r+\Delta r} - [KA_z \partial T / \partial z]_{z+\Delta z} \\ \dot{W}_{out} &= -[DA_r \partial \rho_w / \partial r]_{r+\Delta r} - [DA_z \partial \rho_w / \partial z]_{z+\Delta z} \\ h_w &= \text{enthalpy of the water vapor leaving the system, and} \\ T &= \text{temperature of the air-water vapor mixture} \end{aligned}$$

Substituting the equations for the individual terms into 2-13, the expression for energy transfer out of the system becomes:

$$\begin{aligned}\dot{E}_{out} = & - \left[K(2\pi r \Delta z) \frac{\partial T}{\partial r} \right]_{r+\Delta r} - \left[K(2\pi r \Delta r) \frac{\partial T}{\partial z} \right]_{z+\Delta z} \\ & - \left[Dh_w(2\pi r \Delta z) \frac{\partial \rho_w}{\partial r} \right]_{r+\Delta r} - \left[Dh_w(2\pi r \Delta r) \frac{\partial \rho_w}{\partial z} \right]_{z+\Delta z}\end{aligned}\quad (2-14)$$

The thermal conductivity is known to be a function of temperature. However, as was the case for the diffusion coefficient, this property was assumed to be constant since large variations in temperature were not expected.

$\dot{E}_{gen}$ is the rate of energy generated within the system and is a function of the system volume. Like the mass generation term, it is usually expressed as a rate per unit volume. In addition, the generation of mass (w''') within the system will result in a change in energy due to the change in enthalpy. Because of this fact, an additional term must be included in the energy balance:

$$\dot{E}_{gen} = Vg''' + Vh_w w''' = 2\pi r \Delta r \Delta z (g''' + h_w w''') \quad (2-15)$$

where:

g''' = rate of energy generation per unit volume

w''' = rate of mass generation per unit volume, and

h_w = enthalpy of water vapor at control volume temperature

Note that an assumption was made that the temperature of the water vapor present in the volume is the same as the temperature of the control volume. This essentially requires that the air-water vapor mixture be at the same temperature. Since diffusion rates for water vapor in air are generally very low, this assumption should not introduce significant error.

$\dot{E}_{\text{stor}}$ is the rate of energy stored within the system and is a function of the volume of the system and the specific heat of the system material. Energy may be stored in both the air and the water vapor within the system:

$$\dot{E}_{\text{stor}} = \dot{E}_{\text{stor}_{\text{air}}} + \dot{E}_{\text{stor}_{\text{H}_2\text{O}}} = \rho_a c_a V \frac{\partial T}{\partial t} + \frac{\partial}{\partial t} [\rho_w V h_w] \quad (2-16)$$

where:

- ρ_a = mass concentration of the air
- ρ_w = mass concentration of the water vapor
- c_a = specific heat of the air
- T = temperature, and
- t = time

The second term in 2-15 can be expanded using the product rule as follows:

$$\frac{\partial}{\partial t} (\rho_w V h_w) = \rho_w V \left(\frac{\partial h_w}{\partial T} \right) \frac{\partial T}{\partial t} + V h_w \frac{\partial \rho_w}{\partial t} \quad (2-17)$$

but:

$$\partial h_w / \partial T = \text{specific heat of water vapor } (c_w),$$

therefore:

$$\frac{\partial}{\partial t} (\rho_w V h_w) = V \left[\rho_w c_w \frac{\partial T}{\partial t} + h_w \frac{\partial \rho_w}{\partial t} \right] \quad (2-18)$$

Substituting this result into 2-15:

$$\dot{E}_{\text{stor}} = (2\pi r \Delta r \Delta z) \left[(\rho_a c_a + \rho_w c_w) \frac{\partial T}{\partial t} + h_w \frac{\partial \rho_w}{\partial t} \right] \quad (2-19)$$

Substituting 2-12, 2-14, 2-15, and 2-19 into 2-11 and dividing through by the volume $2\pi r \Delta r \Delta z$:

$$\begin{aligned} & r \left[(\rho_a c_a + \rho_w c_w) \frac{\partial T}{\partial t} + h_w \frac{\partial \rho_w}{\partial t} \right] - r \left[g'''' + h_w w'''' \right] \\ & - \left\{ \frac{K \left[r \frac{\partial T}{\partial r} \right]_{r+\Delta r} - K \left[r \frac{\partial T}{\partial r} \right]_r}{\Delta r} + \frac{K \left[r \frac{\partial T}{\partial z} \right]_{z+\Delta z} - K \left[r \frac{\partial T}{\partial z} \right]_z}{\Delta z} \right\} \\ & - \left\{ \frac{D \left[r h_w \frac{\partial \rho_w}{\partial r} \right]_{r+\Delta r} + D \left[r h_w \frac{\partial \rho_w}{\partial r} \right]_r}{\Delta r} + \frac{D \left[r h_w \frac{\partial \rho_w}{\partial z} \right]_{z+\Delta z} - D \left[r h_w \frac{\partial \rho_w}{\partial z} \right]_z}{\Delta z} \right\} \\ & = 0 \end{aligned} \quad (2-20)$$

Taking limits as Δr and Δz approach zero:

$$\begin{aligned}
 & r \left[(\rho_a c_a + \rho_w c_w) \frac{\partial T}{\partial t} + h_w \frac{\partial \rho_w}{\partial t} \right] - r(g'''' + h_w w''') \\
 & - K \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) - K \frac{\partial}{\partial z} \left(r \frac{\partial T}{\partial z} \right) - D \frac{\partial}{\partial r} \left(r h_w \frac{\partial \rho_w}{\partial r} \right) \\
 & - D \frac{\partial}{\partial z} \left(r h_w \frac{\partial \rho_w}{\partial z} \right) = 0
 \end{aligned} \tag{2-21}$$

Expanding the last two terms in 2-21 using the product and chain rules, the equation for conservation of energy may be written as follows:

$$\begin{aligned}
 & r \left[(\rho_a c_a + \rho_w c_w) \frac{\partial T}{\partial t} + h_w \frac{\partial \rho_w}{\partial t} \right] - r(g'''' + h_w w''') - K \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) \\
 & - K \frac{\partial}{\partial z} \left(r \frac{\partial T}{\partial z} \right) - D h_w \frac{\partial}{\partial r} \left(r \frac{\partial \rho_w}{\partial r} \right) - D c_w r \frac{\partial \rho_w}{\partial r} \left(\frac{\partial T}{\partial r} \right) \\
 & - D h_w \frac{\partial}{\partial z} \left(r \frac{\partial \rho_w}{\partial z} \right) - D c_w r \frac{\partial \rho_w}{\partial z} \left(\frac{\partial T}{\partial z} \right) = 0
 \end{aligned} \tag{2-22}$$

Solution of Governing Equations

Solution of the governing equations involved a combination of algebraic manipulations and numerical analysis. The nature of the problem was particularly suited to the finite element method which has rapidly gained prominence in recent years.

Algebraic manipulations. Examination of the governing equations reveals an interesting condition which was useful in the solution process. The mass equation (2-9) is independent of any energy terms. The energy equation (2-22), however, is coupled with mass because a change in enthalpy is associated with the transfer or generation of mass. Using this information, the mass equation can be solved first and the results substituted into the energy equation for purposes of simplification. From equation 2-9,

$$\frac{\partial \rho_w}{\partial t} = w'''' + \frac{1}{r} D \frac{\partial}{\partial r} \left(r \frac{\partial \rho_w}{\partial r} \right) + \frac{1}{r} D \frac{\partial}{\partial z} \left(r \frac{\partial \rho_w}{\partial z} \right) \quad (2-23)$$

Substitution of 2-23 into 2-22 yields the following simplified energy equation:

$$\begin{aligned} (\rho_a c_a + \rho_w c_w) \frac{\partial T}{\partial t} - g'''' - K \frac{\partial}{\partial r} \left(r \frac{\partial T}{\partial r} \right) - K \frac{\partial}{\partial z} \left(r \frac{\partial T}{\partial z} \right) \\ - D c_w \frac{\partial \rho_w}{\partial r} \left(\frac{\partial T}{\partial r} \right) - D c_w \frac{\partial \rho_w}{\partial z} \left(\frac{\partial T}{\partial z} \right) = 0 \end{aligned} \quad (2-24)$$

In reality, the diffusion of heat and mass occurs simultaneously, and the most desirable solution would be to solve the conservation equations simultaneously. The simplified procedure used above introduces some

error because it essentially uses the results from the mass equation for a given time to update the energy equation at the same time. This implies that the mass is constant for the duration of the time step. If the time steps were not too large, this assumption would be reasonable. Therefore, care should be taken in selecting the times for which solutions are desired.

Finite element analysis. The finite element method is a numerical analysis technique for obtaining approximate solutions to a wide variety of problems. The need for such a method arises because of the impossibility of obtaining exact analytical solutions to non-standard problems. The basis of the method is to reduce a problem with an infinite number of unknowns to one of a finite nature by dividing the solution region into elements. The unknown variables are then expressed in terms of approximating functions within each element (Huebner, 1975). The following list summarizes in general terms the steps involved in using the finite element method (Huebner, 1975):

1. subdivide the solution region
2. select interpolation functions
3. find the element properties
4. assemble the element properties to obtain system equations,
and
5. solve the system equations

Element geometry. For two dimensional problems, the triangle is a particularly useful shape because groups of triangles can be used to represent relatively complex geometries accurately (Zienkiewicz and Morgan, 1983). In addition, the properties of triangular elements are well known. For these reasons, the three-node triangular element geometry was chosen for this analysis. A typical element of volume generated by revolving such an element about the z-axis is shown in Figure 2. Notice that the nodes are lettered in counter-clockwise direction. This procedure is primarily used to maintain a sign convention and overall consistency throughout the development of the element equations.

Interpolation functions. The choice of the interpolation functions used to approximate the unknown nodal values depends upon the number of nodes assigned to the element, the nature and number of unknowns at each node, and continuity requirements imposed at the nodes and along element boundaries (Huebner, 1975). For the linear triangular element chosen for this problem there were two unknowns at each of the three nodes--concentration of water vapor and temperature. Because they are easy to manipulate mathematically, polynomials are the most common type of interpolation function (Huebner, 1975). The simplest form is the linear polynomial which may be expressed as follows:

$$N(x) = a_0 + a_1x \quad (2-25)$$

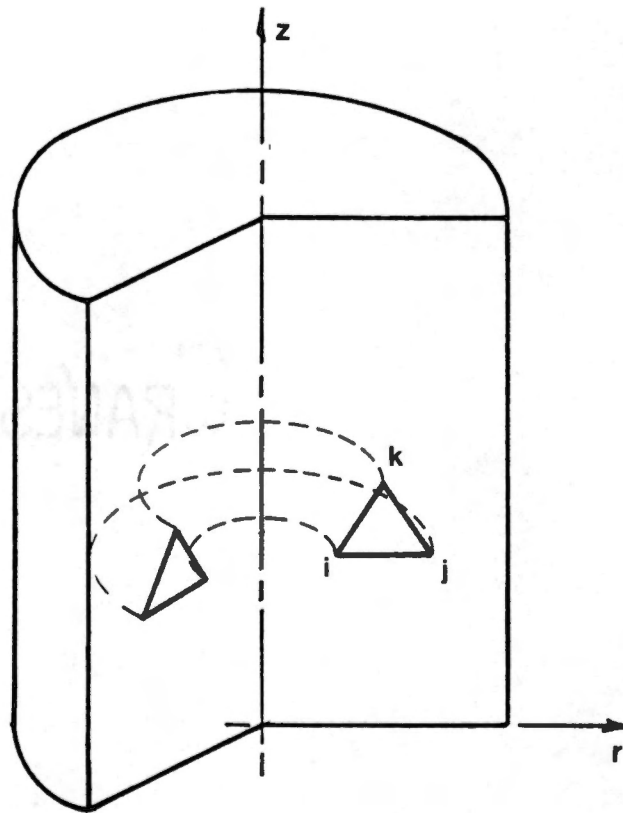


Figure 2. Typical Element of Volume
Showing a Three-Node Linear
Triangle.

For the two dimensional radially axi-symmetric system, the interpolation function for nodal concentration takes the following form:

$$N(r,z) = a_0 + a_1 r + a_2 z \quad (2-26)$$

Referring to Figure 2, the value of concentration for the element can be approximated by interpolating among the values at the three nodes i, j, and k:

$$\rho_w \cong \bar{\rho}^e = N_i \rho_i + N_j \rho_j + N_k \rho_k + \sum N_n^e \rho_n^e(t) \quad (2-27)$$

where:

$\bar{\rho}^e$ = the approximate value of concentration in the element

ρ_n^e = the concentration of node n which is a function of time

N_n = the interpolation functions for node n of a particular element

The interpolation functions expressed in terms of the three nodes of a triangular element are written as follows:

$$N_i^e = \frac{1}{2A} (a_i + b_i r + c_i z) \quad (2-28a)$$

$$N_j^e = \frac{1}{2A} (a_j + b_j r + c_j z) \quad (2-28b)$$

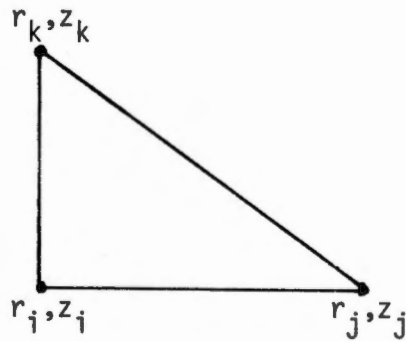
$$N_k^e = \frac{1}{2A} (a_k + b_k r + c_k z) \quad (2-28c)$$

where:

A = area of an element in the r - z plane

a_n, b_n, c_n = constants for a given element that can be expressed in terms of the element's nodal position

As an example, consider the triangular element shown below.



The area of the element is given by the following formula:

$$A = \frac{1}{2} \left| r_i (z_j - z_k) + r_j (z_k - z_i) + r_k (z_i - z_j) \right| \quad (2-29)$$

The constants for the three nodes of the element are expressed in terms of the position coordinates r and z :

$$a_i = r_j z_k - r_k z_j; \quad a_j = r_k z_i - r_i z_k; \quad a_k = r_i z_j - r_j z_i \quad (2-30a)$$

$$b_i = z_j - z_k; \quad b_j = z_k - z_i; \quad b_k = z_i - z_j \quad \text{and} \quad (2-30b)$$

$$c_i = r_k - r_j; \quad c_j = r_i - r_k; \quad c_k = r_j - r_i \quad (2-30c)$$

The approximate value of concentration for this element can then be written in matrix form:

$$\bar{\rho}_w^e = \begin{bmatrix} N_i^e & N_j^e & N_k^e \end{bmatrix} \begin{Bmatrix} \rho_i^e \\ \rho_j^e \\ \rho_k^e \end{Bmatrix} = \begin{bmatrix} N_n \end{bmatrix}^e \begin{Bmatrix} \rho_n \end{Bmatrix}^e \quad (2-31)$$

Minimization technique. The governing equations must be valid for any element. Substitution of the approximations for nodal concentrations and temperatures in the respective equations introduces error, and the equations will, in general, no longer be satisfied. The solutions for concentrations and temperatures which minimize this error are desired. Several minimization techniques are available for this purpose, and the selection of a method depends upon the nature of the problem. The Galerkin method, which is a weighted residual approximation, was chosen. This method specifies that the residual, or error introduced by approximating the unknowns, vanishes in an average sense over the entire solution domain (Huebner, 1975). Specifically, the integral of the product of the residual, R , and the approximating functions, N , over the volume of the element must vanish:

$$\int_{V^e} R N_n^e dV = 0 \quad \text{for } n = i, j, k \quad (2-32)$$

If the residual were to be replaced by the differential equation it represents, the approximating function for the mass equation would be:

$$\int_{V^e} \left[\frac{\partial \bar{\rho}_w}{\partial t} - w'''' - D \frac{\partial^2 \bar{\rho}_w}{\partial r^2} - \frac{D}{r} \frac{\partial \bar{\rho}_w}{\partial r} - D \frac{\partial^2 \bar{\rho}_w}{\partial z^2} \right] N_n dV = 0$$

for $n = i, j, k$ (2-33)

Similarly, for the energy equation:

$$\int_{V^e} \left[(\rho_a c_a + \bar{\rho}_w c_w) \frac{\partial \bar{T}}{\partial t} - g'''' - K \frac{\partial^2 \bar{T}}{\partial r^2} - \frac{K}{r} \frac{\partial \bar{T}}{\partial r} - K \frac{\partial^2 \bar{T}}{\partial z^2} - D c_w \frac{\partial \bar{\rho}_w}{\partial r} \frac{\partial \bar{T}}{\partial r} - D c_w \frac{\partial \bar{\rho}_w}{\partial z} \frac{\partial \bar{T}}{\partial z} \right] N_n dV = 0$$

for $n = i, j, k$ (2-34)

Using $\bar{\rho}_w = [N_n] \{ \rho_n \}$, $\bar{T} = [N_n] \{ T_n \}$, and $dV = 2\pi r dr dz$:

$$\int_z \int_r 2\pi r \left[\frac{\partial}{\partial t} ([N_n] \{ \rho_n \}) - w'''' - D \frac{\partial^2}{\partial r^2} ([N_n] \{ \rho_n \}) - \frac{D}{r} \frac{\partial}{\partial r} ([N_n] \{ \rho_n \}) - D \frac{\partial^2}{\partial z^2} ([N_n] \{ \rho_n \}) \right] N_n dr dz = 0 \quad \text{for } n = i, j, k \quad (2-35)$$

for the mass equation, and:

$$\begin{aligned}
 & \iint_{z,r} 2\pi r \left\{ \left[\rho_a c_a + [N_n] \{ \rho_n \} c_w \right] \frac{\partial}{\partial t} ([N_n] \{ T_n \}) - g'''' - K \frac{\partial^2}{\partial r^2} ([N_n] \{ T_n \}) \right. \\
 & - \frac{K}{r} \frac{\partial}{\partial r} ([N_n] \{ T_n \}) - K \frac{\partial^2}{\partial z^2} ([N_n] \{ T_n \}) - D c_w \frac{\partial}{\partial r} ([N_n] \{ \rho_n \}) \frac{\partial}{\partial r} ([N_n] \{ T_n \}) \\
 & \left. - D c_w \frac{\partial}{\partial r} ([N_n] \{ \rho_n \}) \frac{\partial}{\partial z} ([N_n] \{ T_n \}) \right\} N_n \, dr dz = 0
 \end{aligned}$$

$$\text{for } n = i, j, k \quad (2-36)$$

for the energy equation. Note that the same interpolating functions were used in both equations. Since the element properties (i.e., coordinates, areas, and volumes) are dependent only on the grid chosen for the problem, the values of the element properties are the same for both equations.

Evaluation of integrals. Each of the terms in 2-35 and 2-36 was evaluated and written in a form suitable for coding into a computer. Evaluations were performed term by term. The nodal values of concentration and temperature are functions of time only, while the interpolation functions are functions of position only. Consequently, the terms in 2-35 and 2-36 can be simplified:

$$\frac{\partial}{\partial t}([N_n] \{\rho_n\}) = [N_n] \left\{ \frac{\partial \rho_n}{\partial t} \right\} = [N_n] \{\dot{\rho}_n\} \quad (2-37a)$$

$$\frac{\partial}{\partial t}([N_n] \{T_n\}) = [N_n] \left\{ \frac{\partial T_n}{\partial t} \right\} = [N_n] \{\dot{T}_n\} \quad (2-37b)$$

$$\frac{\partial}{\partial r}([N_n] \{\rho_n\}) = \frac{\partial}{\partial r}([N_n]) \{\rho_n\} ; \quad \frac{\partial}{\partial z}([N_n] \{\rho_n\}) = \frac{\partial}{\partial z}([N_n]) \{\rho_n\} \quad (2-37c)$$

$$\frac{\partial}{\partial r}([N_n] \{T_n\}) = \frac{\partial}{\partial r}([N_n]) \{T_n\} ; \quad \frac{\partial}{\partial z}([N_n] \{T_n\}) = \frac{\partial}{\partial z}([N_n]) \{T_n\} \quad (2-37d)$$

The derivatives of the interpolation functions may be written as follows:

$$\frac{\partial}{\partial r} [N_n] = \frac{\partial}{\partial r} [N_i \ N_j \ N_k] = \frac{1}{2A} [b_i \ b_j \ b_k] \quad (2-38a)$$

$$\frac{\partial}{\partial z} [N_n] = \frac{\partial}{\partial z} [N_i \ N_j \ N_k] = \frac{1}{2A} [c_i \ c_j \ c_k] \quad (2-38b)$$

Since these terms are functions of either r or z :

$$\int_z \int_r 2\pi r dr dz = \int_{V^e} dV = \int_{V^e} 2\pi \bar{r} dA = 2\pi \bar{r} A \quad (2-39)$$

where:

$$\bar{r} = \frac{(r_i + r_j + r_k)}{3}$$

Matrix notation. Once all the terms in the governing equations have been evaluated, the next step is to express them in a form suitable for computer coding. Since the finite element method is based on subdivision of the solution region, and since the interpolation functions allow expression of the unknown concentrations and temperatures in terms of the nodal values, matrix notation was the logical choice. A summary of the matrix expressions for each of the terms in the governing equations is included in Appendix 1.

CHAPTER III

COMPUTER PROGRAM

Overview of the Program

A FORTRAN (FORTRAN H extended enhanced compiler) program was written using the matrix expressions for the governing equations. The program was developed in the most general manner possible to allow maximum flexibility in application. The main section is essentially a generalized core which includes the input of data, formation of influence matrices for the mass equation and the constant portions of the energy equation, matrix manipulations, integration subroutines, and the output of results. Matrix manipulations and integration were performed by IMSL FORTRAN subroutines. The integration subroutine used was DVERK, a variable order, variable step Runge-Kutta technique for initial value problems. A summary of the IMSL subroutines used is included in Appendix 2.

In order to make the program as general as possible, the coding for generation of mass and energy was placed in user-specified subroutines. This would allow flexibility in the use of the model for a variety of problems. As mentioned before, the model does not directly account for changes of phase, however, the user may supply the appropriate generation of heat and mass which satisfies the energy and mass balances for a particular phase change. While this may appear

to be a deficiency in the model, it was necessary to maintain generality. The model can handle both constant and time-dependent generation of heat and mass. Again, it is the user's responsibility to modify the program to account for these specific applications.

Flow Chart of Program

Flow charts for the main program and the subroutines are shown in Figures 3 through 6. A complete listing of the program and description of the variables and arrays are included in Appendix 3.

The first step in any FORTRAN program is to dimension and declare variables and arrays. The IMSL subroutines used for integration and matrix manipulations require double precision representation. Another peculiarity of these library subroutines is that the matrices have to be dimensioned exactly to the number of nodes and elements used in the grid chosen for a problem. Therefore, the dimension statements in the main program as well as some of the subroutines must be redimensioned for each grid.

The input data supplied from a separate program are read in the next sections of the program. These data include information about the grid being used (i.e., number of nodes, number of elements, element numbers and nodal coordinates), specified boundary conditions, initial conditions, values of constants, integration time step information, and output specifications. The option of partitioning the problem into two integration intervals with variable time steps is available. This allows small integration steps to be specified for the period of

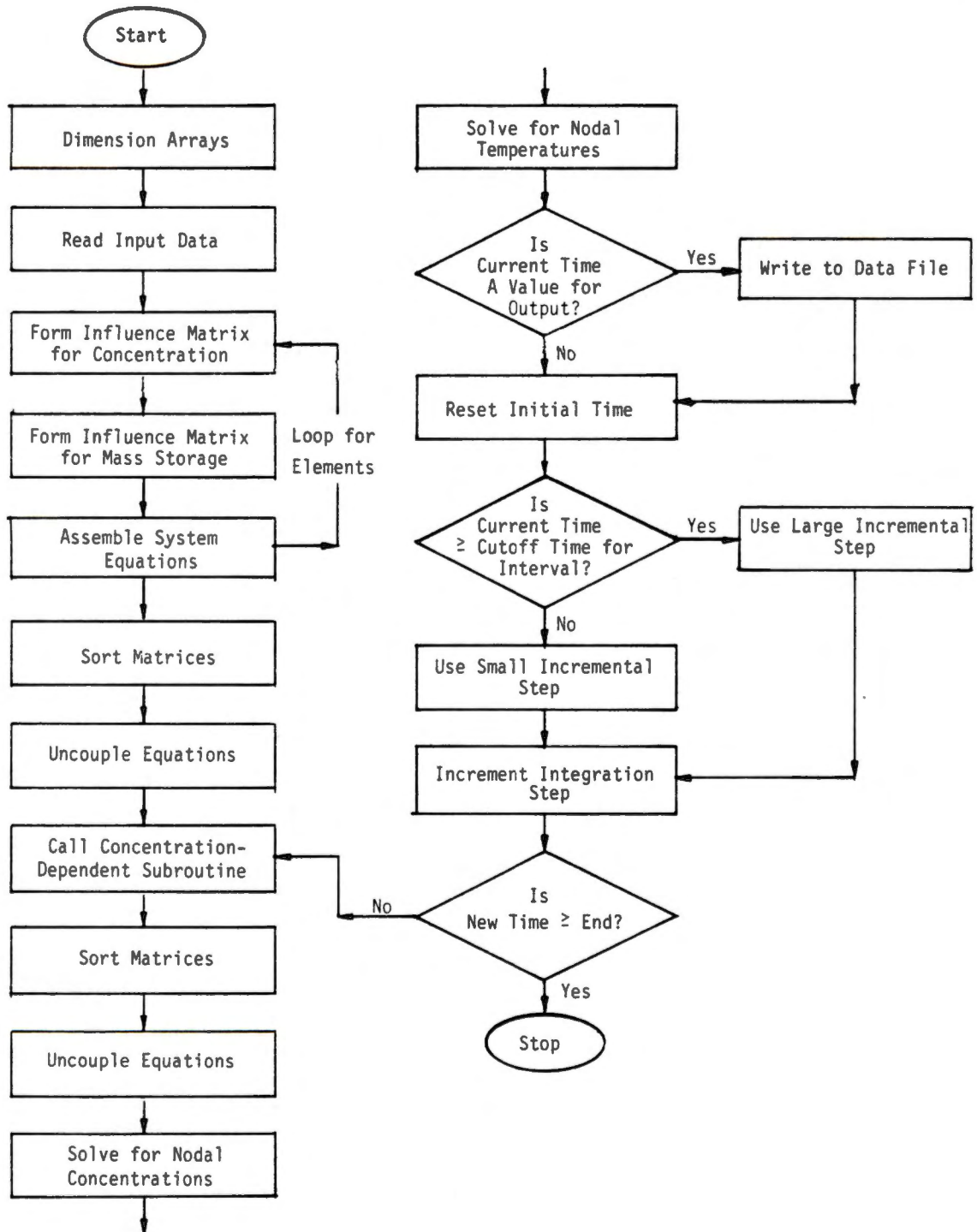


Figure 3. Flow Chart of Main Program.

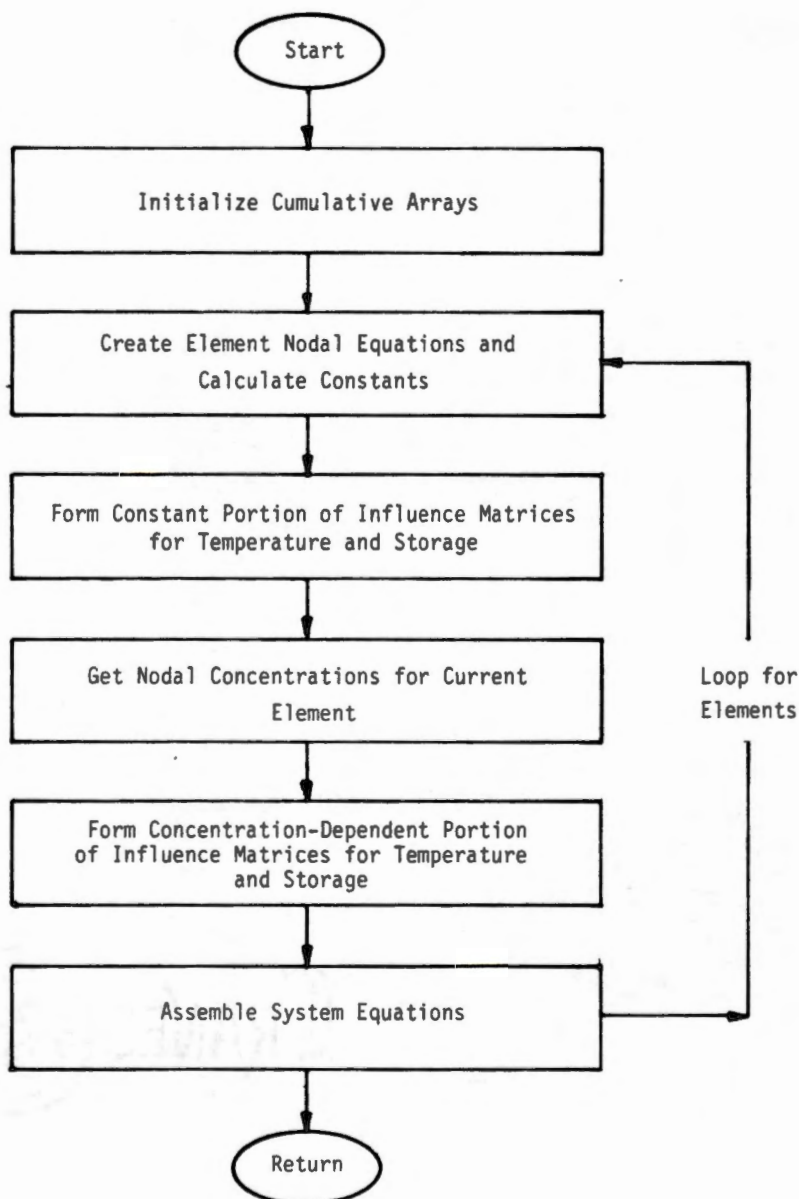


Figure 4. Flow Chart of Concentration-Dependent Subroutine.

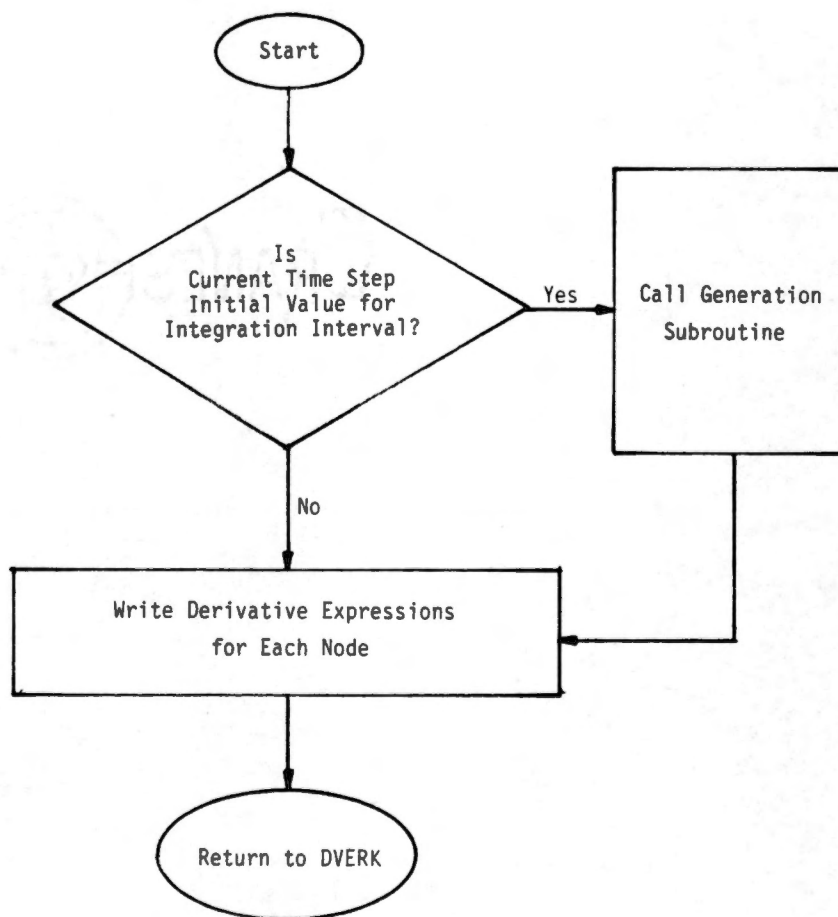


Figure 5. Flow Chart of User-Supplied Subroutine for Derivative Expressions Used By Integration Subroutine.

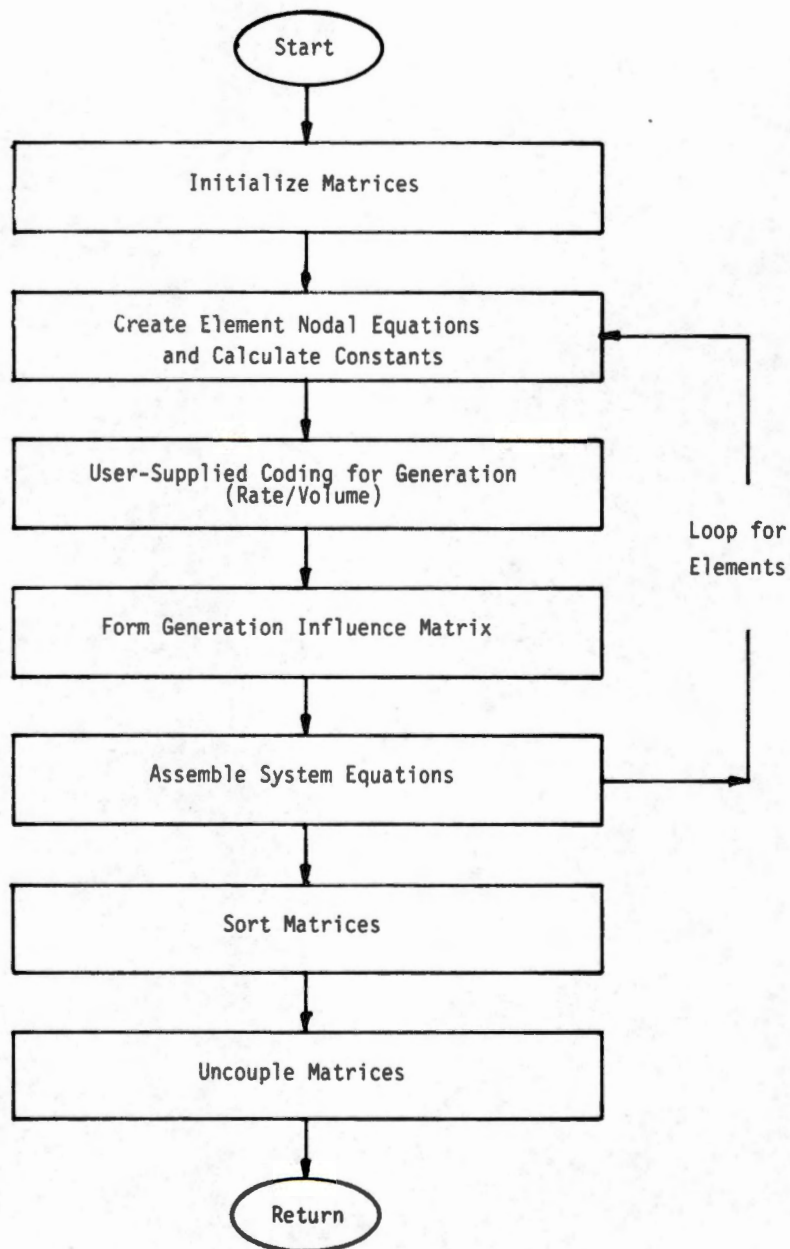


Figure 6. Flow Chart of User-Specified Generation Subroutines.

time when the most changes are expected, after which larger steps may be used when the rate of change is slower and accuracy requirements are not so stringent. The user may also input the times for which output is desired. The only stipulation is that these times must correspond with a time step at which integration is performed.

The next sections deal with formation of the element influence matrices for the mass equation and part of the energy equation. An influence matrix is formed for each term in the governing equation (i.e., storage, generation). Since the mass equation contains no energy terms these calculations are performed only once for a specific problem. Once the equations are written in terms of the three nodes of an element, they are assembled into a master matrix. The dimension of these master influence matrices is equal to the number of elements.

Since concentration and temperature are usually specified at the boundaries, some of the respective nodal values are known and need not be computed. Therefore, the next section is a sorting procedure designed to partition the master influence matrices. New matrices containing only the unknown values are formed for use in the solution of unknown nodal values.

Matrix manipulations were used to uncouple the equations. This process utilizes the properties of inversion, multiplication, eigenvalues, and eigenvectors to express the governing equations as a set of first order linear differential equations which could be integrated and solved for unknown nodal concentrations and temperatures. Once accomplished, the integration subroutine is called to perform the actual solution.

Since the energy equation contains terms which depend upon the current concentration, a separate subroutine was used to form the concentration-dependent influence matrices. Nodal concentrations from the current time step are brought into this subroutine in order to update the energy equation. This procedure places a restriction on the selection of time steps because it assumes that the concentrations remain constant for the duration of the time step. The larger the interval, the poorer this assumption becomes.

CHAPTER IV

VERIFICATION OF THE MODEL

Verification of the model was performed in two stages: comparison with analytical solutions, and comparison with experimental data. Both were necessary to verify the accuracy of the coding and to determine the validity of the theory.

Comparison with Analytical Solutions

The classic text Conduction of Heat in Solids (Carslaw and Jaeger, 1959) contains a wealth of solutions to conduction heat transfer problems. Because of the similarities between conduction heat transfer and diffusion, some of these solutions provided an excellent means of checking the accuracy of the computer coding. By comparing results generated by the model with the analytical solutions to classic problems in the text, the coding for conservation of mass and energy could be tested. Two standard problems were especially useful in this process. Both dealt with the flow of heat in an infinite cylinder. The results were presented in dimensionless form so that comparisons could easily be made.

Case One

The first case involved an infinite cylindrical chamber with zero initial conditions (i.e., temperature or concentration) and its

surface maintained at a constant value. Based on the shape of the curves, an appropriate grid was chosen, and the problem was analyzed with the model. The grid used is shown in Figure 7. Note that the solution region was partitioned with non-uniform spacing. The greatest changes occur near the outer boundary, therefore the mesh was graded so that the finest spacing corresponded with this area. Model results for both temperature and concentration were obtained, and the differences between the two were inconsequential. Comparison of simulated and actual results for temperatures are illustrated in Figure 8. Results for concentrations were virtually identical. This problem provided a means of checking the program to ensure that the specified boundary conditions are enforced.

Case Two

The second case involved an infinite cylindrical chamber with internal generation of heat or mass at a constant rate. Initial and surface conditions were zero. The same grid as in the previous case (Figure 7) was used for this problem. Again, the differences between mass and energy results from the model were inconsequential. Comparison of simulated and actual results for temperatures are shown in Figure 9. Results for concentration were once again virtually identical. This case provided a means of checking the coding for the generation subroutines.

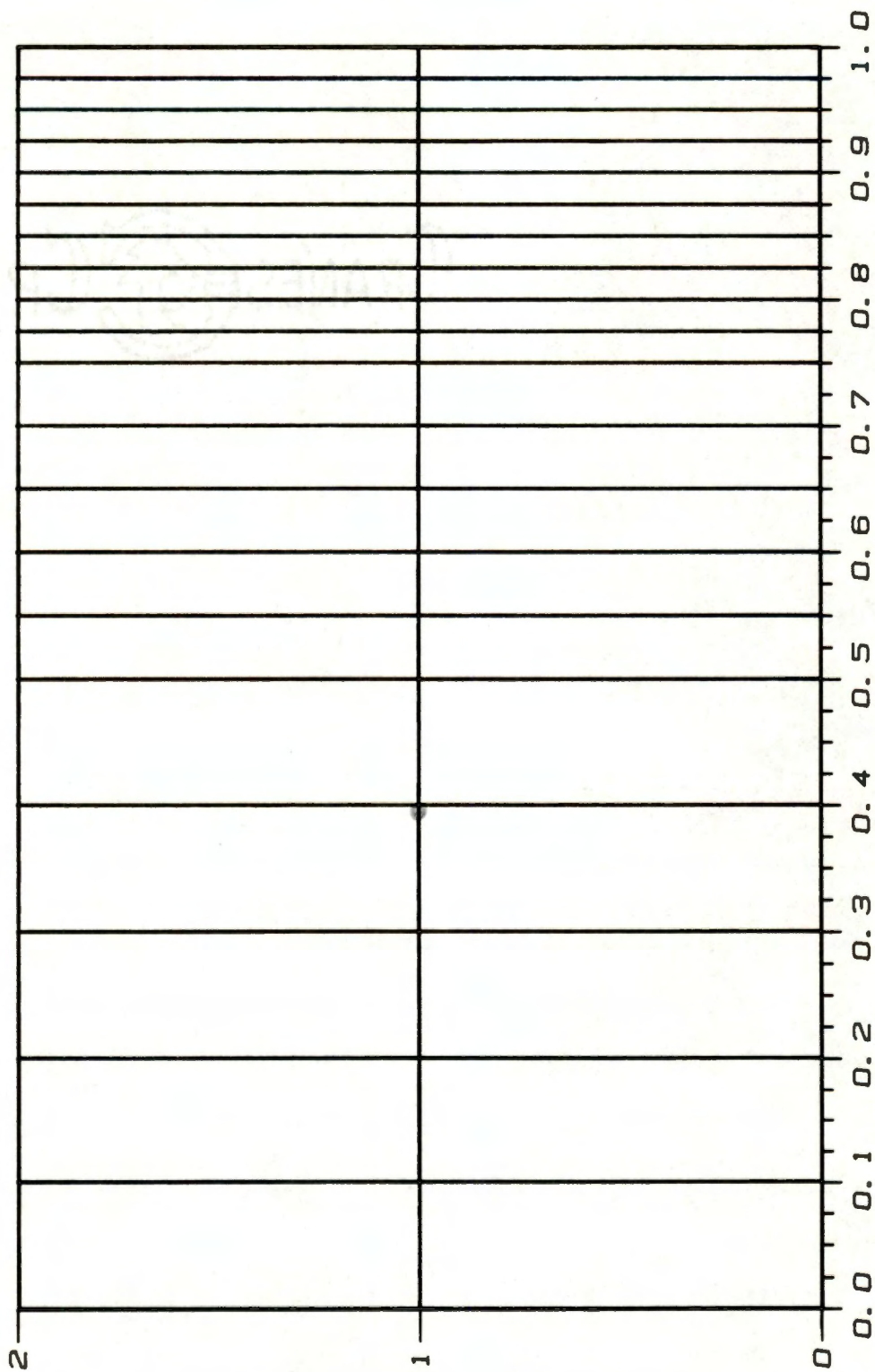


Figure 7. Grid Used in Finite Element Solution for Test Cases.

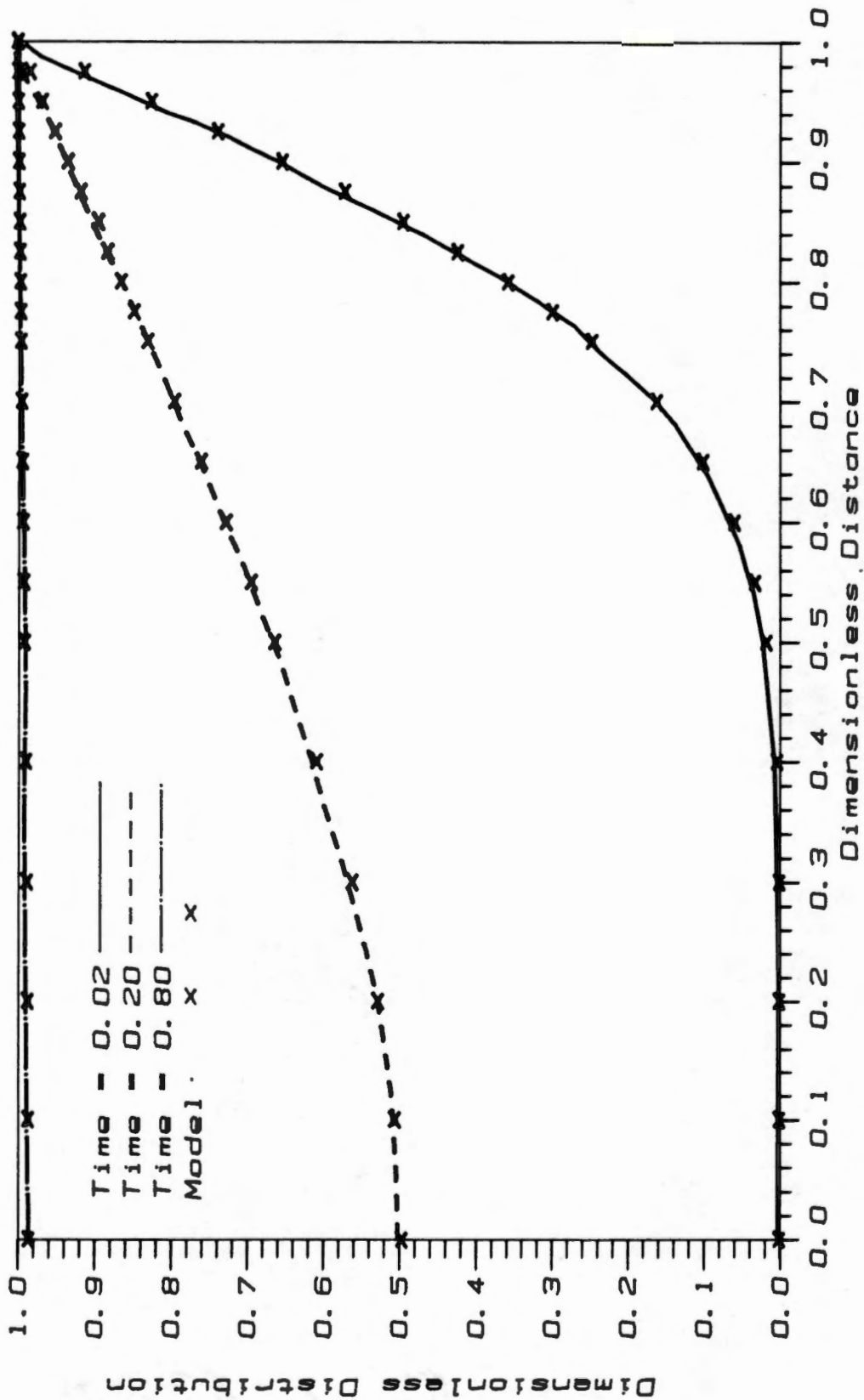


Figure 8. Comparison of Simulated and Analytical Results for Temperature Distribution in a Cylindrical Chamber with Zero Initial Temperature and Specified Boundary Temperature of Unity.

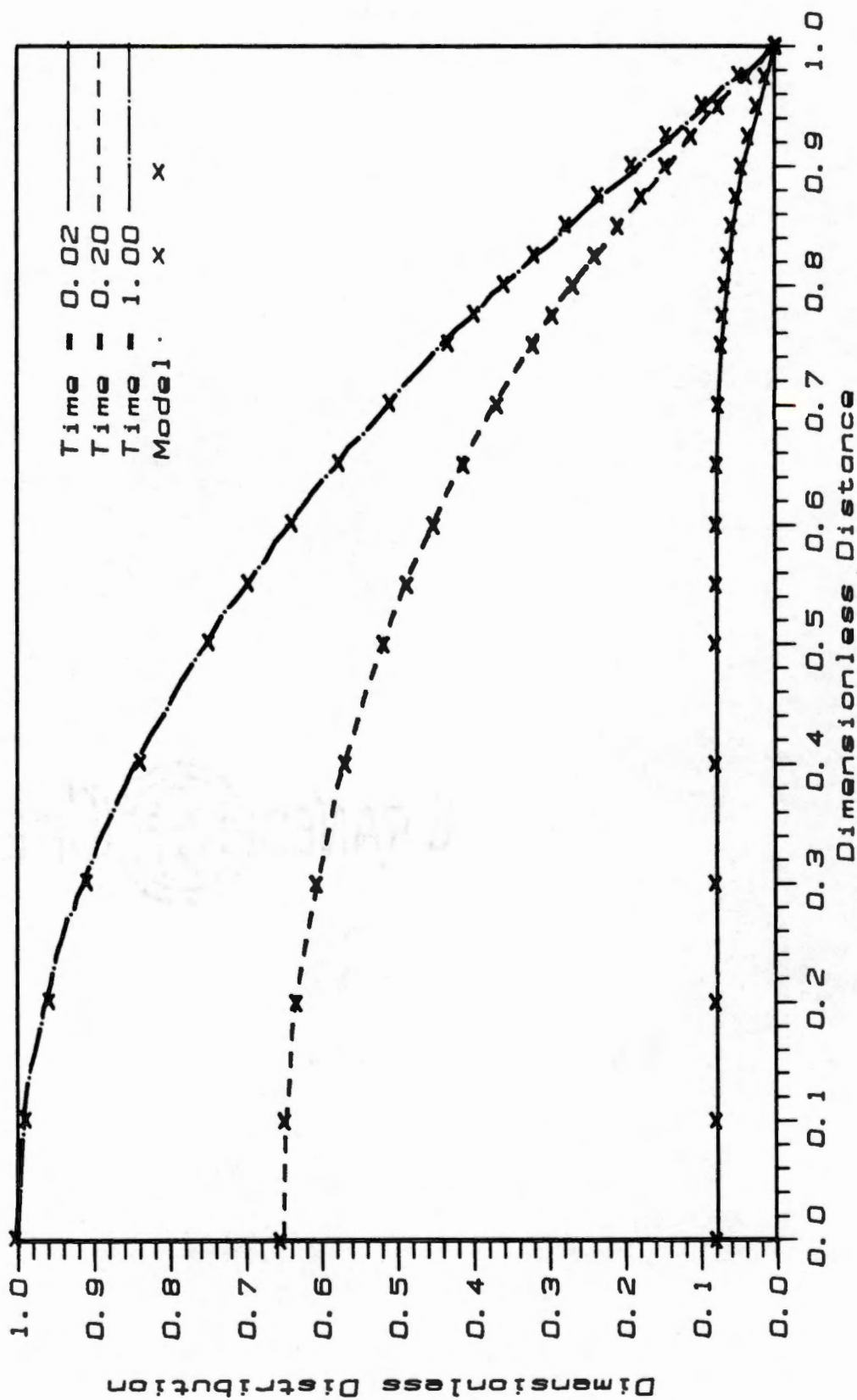


Figure 9. Comparison of Simulated and Analytical Results for Temperature Distribution in a Cylindrical Chamber with Zero Initial and Surface Temperature and Constant Generation.

Comparison with Experimental Data

The preceding discussion dealt with verification of the coding for mass and energy conservation equations. This was necessary to be sure that the equations were accurately transferred into computer coding and to check the overall program logic. An additional verification which dealt with the accuracy of the theory in simulating experimental conditions was necessary. Only after comparing simulated results with actual data could the validity of assumptions made in the development of the model be determined.

Experimental Considerations

The objective of experimental work was to obtain actual data with which simulated results could be compared. Several factors had to be considered in the development of an experiment to meet this objective. The first criterion dealt with the coordinate system used in the derivation of governing equations. In order to make valid comparisons between experimental and simulated results, the control volume used in the actual tests had to possess the same geometry as that used in the model. In addition to the geometry, size of the control volume was important. An ideal case would be a control volume of sufficient size that the boundaries remain unaffected by internal and external disturbances. This was necessary to enforce boundary conditions in the model. Time-dependent boundary conditions could be specified, but at this stage the desire was to maintain simplicity wherever possible.

Another factor was the selection of appropriate instrumentation. Parameters to be measured were temperature and mass concentration of water vapor at various positions in the control volume. Number and location of sensors had to correlate with the grid used to partition the solution region. In addition to the sensors, a data acquisition system was necessary to collect and store information.

Materials and Methods

All experimental work was conducted in the Soil and Water Laboratory in the Agricultural Engineering Building at The University of Tennessee, Knoxville. A cylindrical concrete chamber was used as the control volume. The chamber was 1.52 m high and 5.66 m in diameter. A schematic diagram of the chamber is shown in Figure 10. Note that an irregularity existed in the cylindrical geometry at the top of the tank. An access opening covered with steel plates extended along the central axis. The opening was 0.61 m wide and 5.49 m long. A rectangular concrete beam extended into the top of the tank on either side of the opening. The difference between the actual volume of the tank and that of a true cylinder was only 1 percent so this irregularity was assumed to be insignificant with respect to geometric distortion.

An initial test was performed to determine the uniformity of temperature at the boundaries. Type T thermocouples were installed at the floor--wall and ceiling--wall junctions at 90 degree intervals and at the center. Temperatures were scanned with a Kaye Instruments RAMP (remote analog multiplexing processor) scanner, model 128SS,

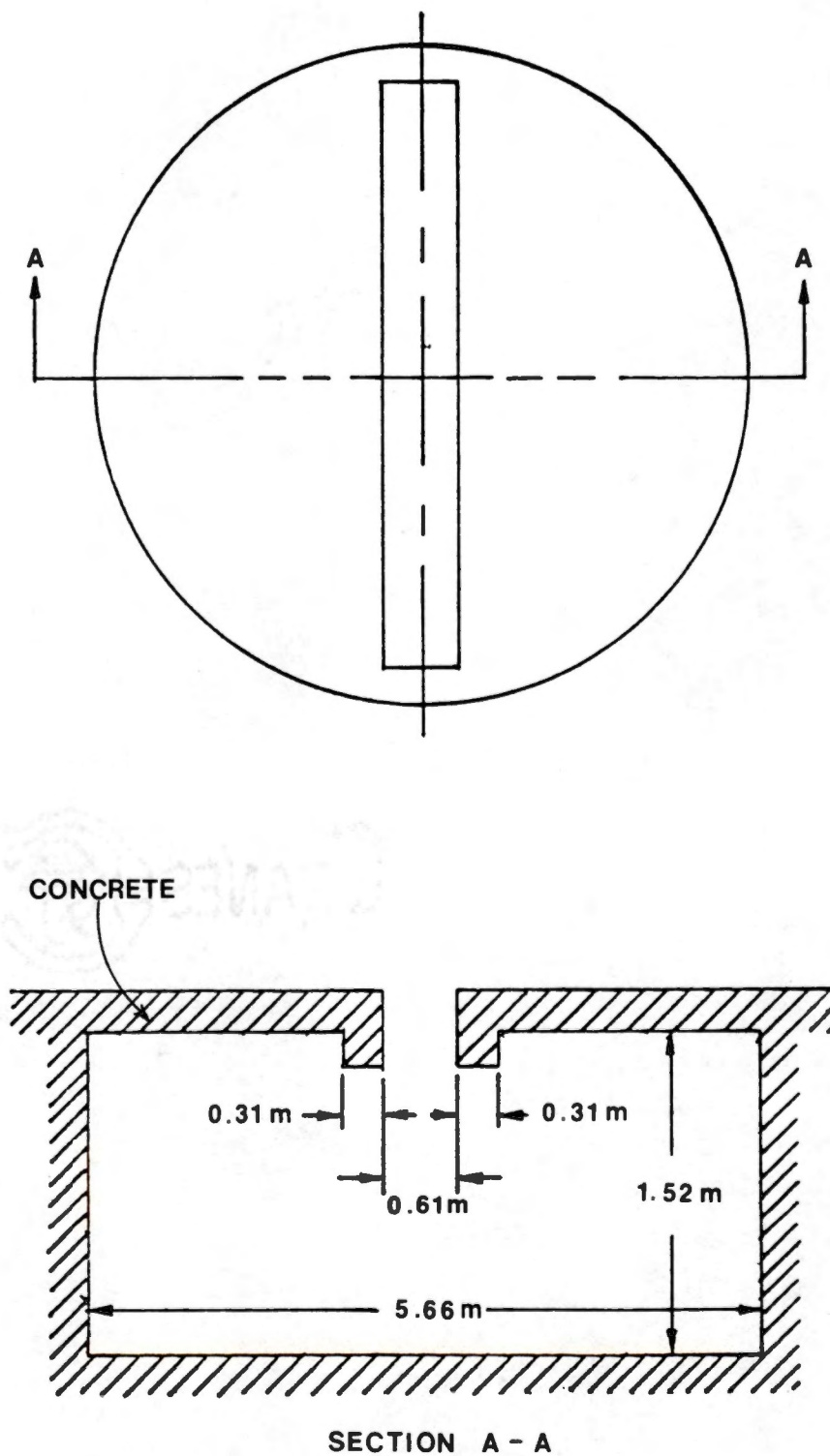


Figure 10. Schematic Diagram of the Concrete Chamber Used as a Control Volume.

interfaced with an IBM Personal Computer. Boundary temperatures were uniform from position to position and nearly constant with time. Additional thermocouples were installed on two orthogonal radii offset 45 degrees from the access opening. This offset was to minimize the number of thermocouple stations in the region of irregular geometry. Seven radial and three vertical positions were used on each leg for purposes of replication. Thermocouple locations are shown in Figure 11.

The mass concentration of water vapor could not be measured directly. It can, however, be calculated using psychrometric properties from the dry bulb temperature and relative humidity. For this reason, hygrothermographs (Weather Measure Corporation, model H-302) were used to monitor temperature and humidity. This provided a second method of temperature measurement. Because of a limited number of hygrothermographs, all seven recorders were placed on one radius. The accuracy gained by incorporating more observations on one radius was felt to be more important than replicating results. Recorder stations are marked with an "x" in Figure 11.

Results and Discussion

In early tests the chamber was initially exposed to ambient conditions by leaving two of the metal plates open. The chamber was then sealed by closing the plates, and temperature and humidity data were monitored for a period of time. Examination of these data revealed that the temperature remained constant while relative humidity increased, rapidly at first, and then slowly approached an equilibrium

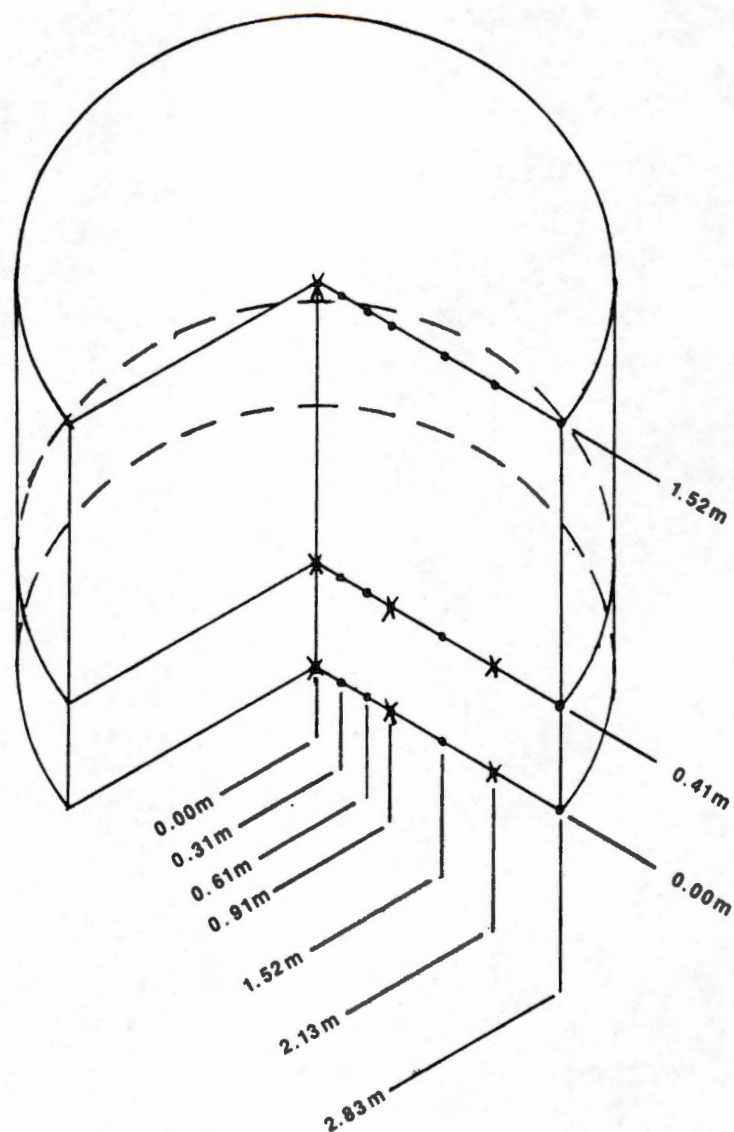


Figure 11. Locations of Sensors in the Chamber -
"." Marks Thermocouple Positions, "x"
Marks Hygrothermograph Locations.

moisture content. These results implied that water vapor was leaking into the chamber. Since the moisture content in the ambient air above the chamber was lower than that inside, the only explanation was that the moisture was being transferred through the concrete. The source and precise location of the leak could not be determined. An attempt was made to stop the leak by lining the inside of the chamber with 6 mil polyurethane plastic. The equilibrium moisture content was lowered slightly, but the leak was not stopped.

Figure 12 shows the increase in moisture content over time at two corresponding positions along the two radii before plastic was installed. The difference between the two curves is small and is probably caused by calibration error. Figure 13 shows the leakage curve for similar initial conditions after the tank was lined with plastic. The effect of the plastic was a decrease in the rate of change and a lowering of the final equilibrium concentration.

The model was used to simulate the change in concentration due to the leak by specifying the boundaries to be at the equilibrium concentration estimated from Figure 12. Specification of temperature or concentration at a boundary node results in a flux at that node. This essentially causes a constant flux boundary condition to be enforced. In this case, the equilibrium concentration was used to estimate the flux due to the leak. The fact that the source and location of the leak could not be determined complicated the simulation. It was not logical to specify any influx from the air above the tank because the interior of the chamber was at a higher concentration than the outside

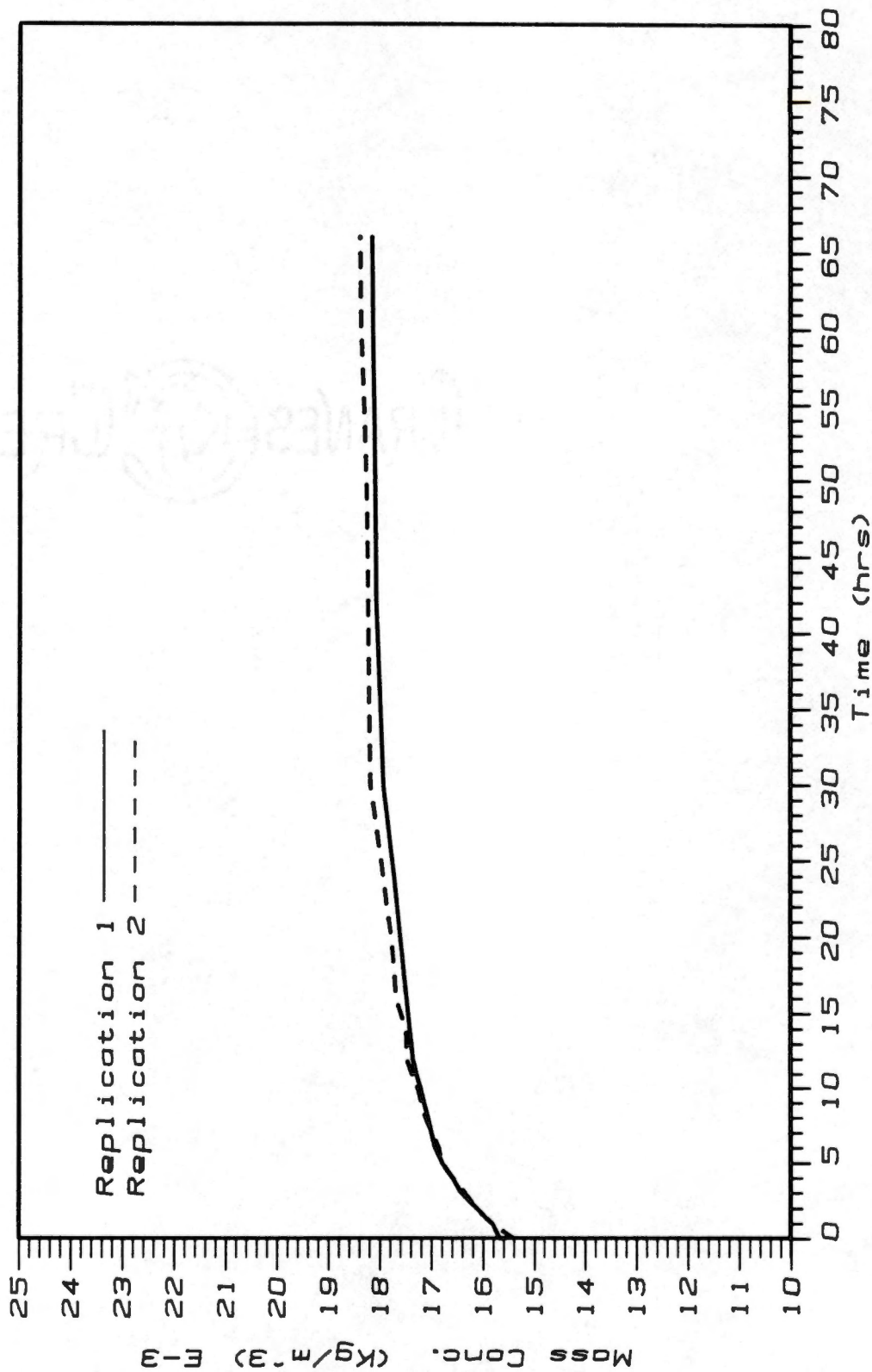


Figure 12. Change in Water Vapor Concentration Over Time at Two Positions in the Chamber Before Plastic Was Installed.

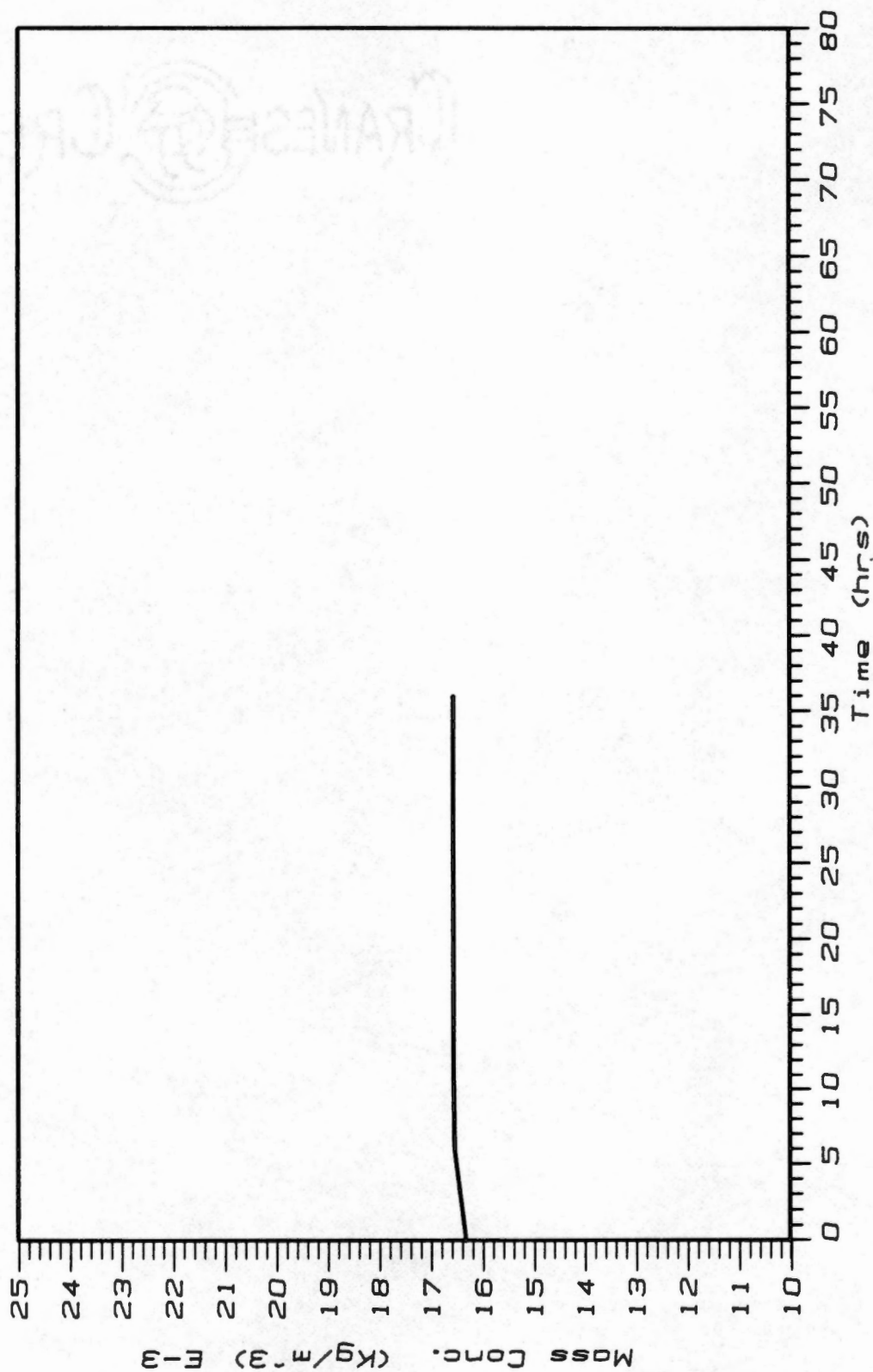


Figure 13. Change in Water Vapor Concentration Over Time After Plastic Was Installed.

air. Several possible combinations involving floor and wall nodes were simulated. The best results were obtained when the leak was assumed to come uniformly through the wall. Comparison of actual and simulated results for one position in the chamber is shown in Figure 14. The model curve (dashed line) shows a 2-hour lag before any increase in concentration occurred. This position was located nearly midway between the wall and the center. The flux was specified to be entering through the wall, and consequently a finite period of time was required to reach this node. A better comparison may be made by removing this time lag in the model curve as shown in Figure 15. The agreement between the two curves is encouraging and indicates that the model is capable of predicting actual phenomena accurately. In reality, however, the leak probably does not occur uniformly through the wall alone. This analysis was not intended to explain the leak, but it does help to verify the theory upon which the model was developed.

An analysis of the sensitivity of the rate of change in concentration to the value of the diffusion coefficient was performed. For the same initial and boundary conditions as before, three different values for the diffusion coefficient of water vapor in air were used. The values were arbitrarily chosen to bracket the published value of $0.093 \text{ m}^2/\text{hr}$ at 26°C . Results were shown in Figure 16. The expected trend of increasing rate for higher diffusion coefficients is obvious. The results indicate that even a 50 percent difference in the value of the diffusion coefficient does not drastically alter the time response of the mass concentration.

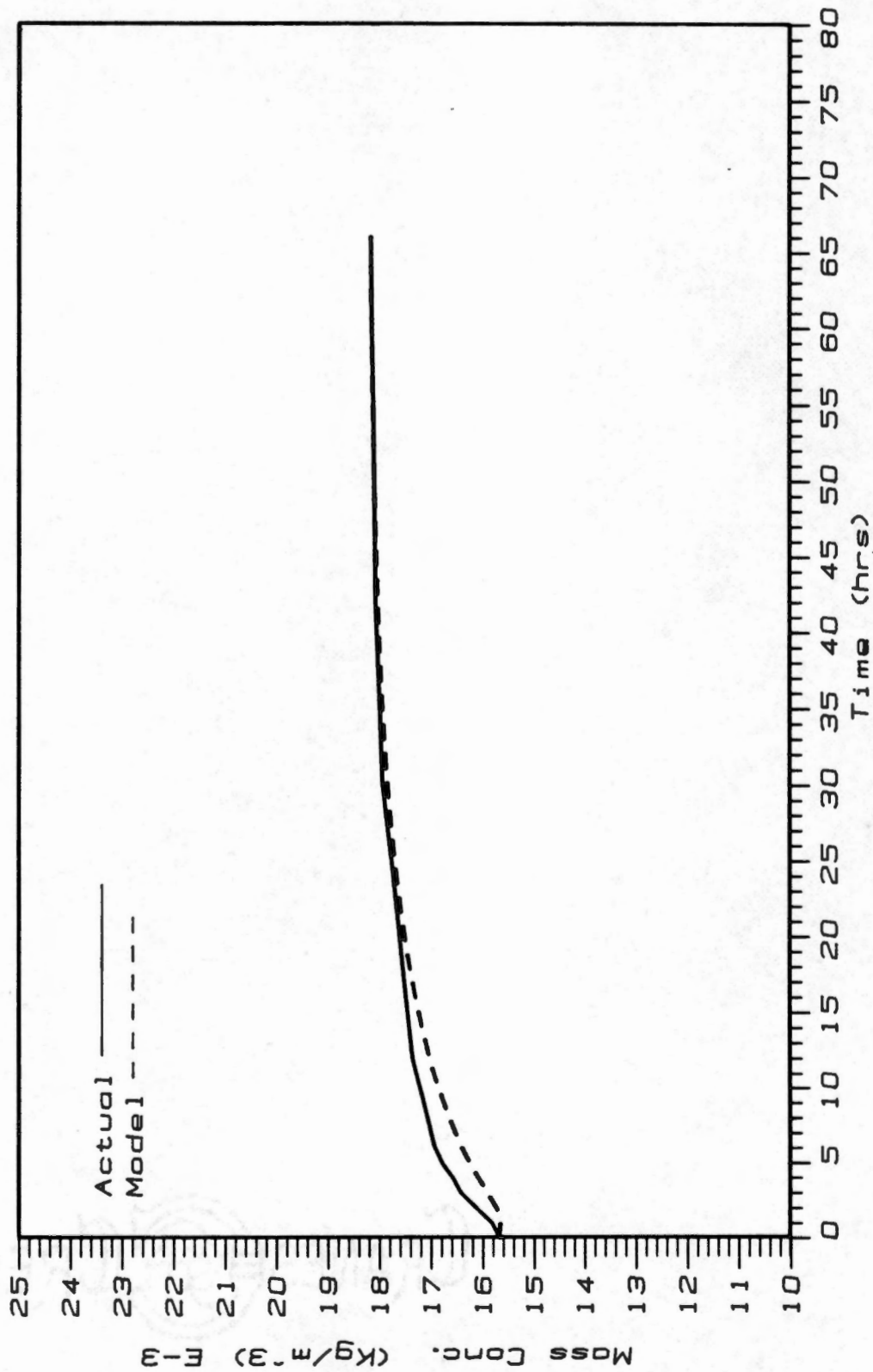


Figure 14. Comparison of Actual and Simulated Results for One Position in the Chamber.

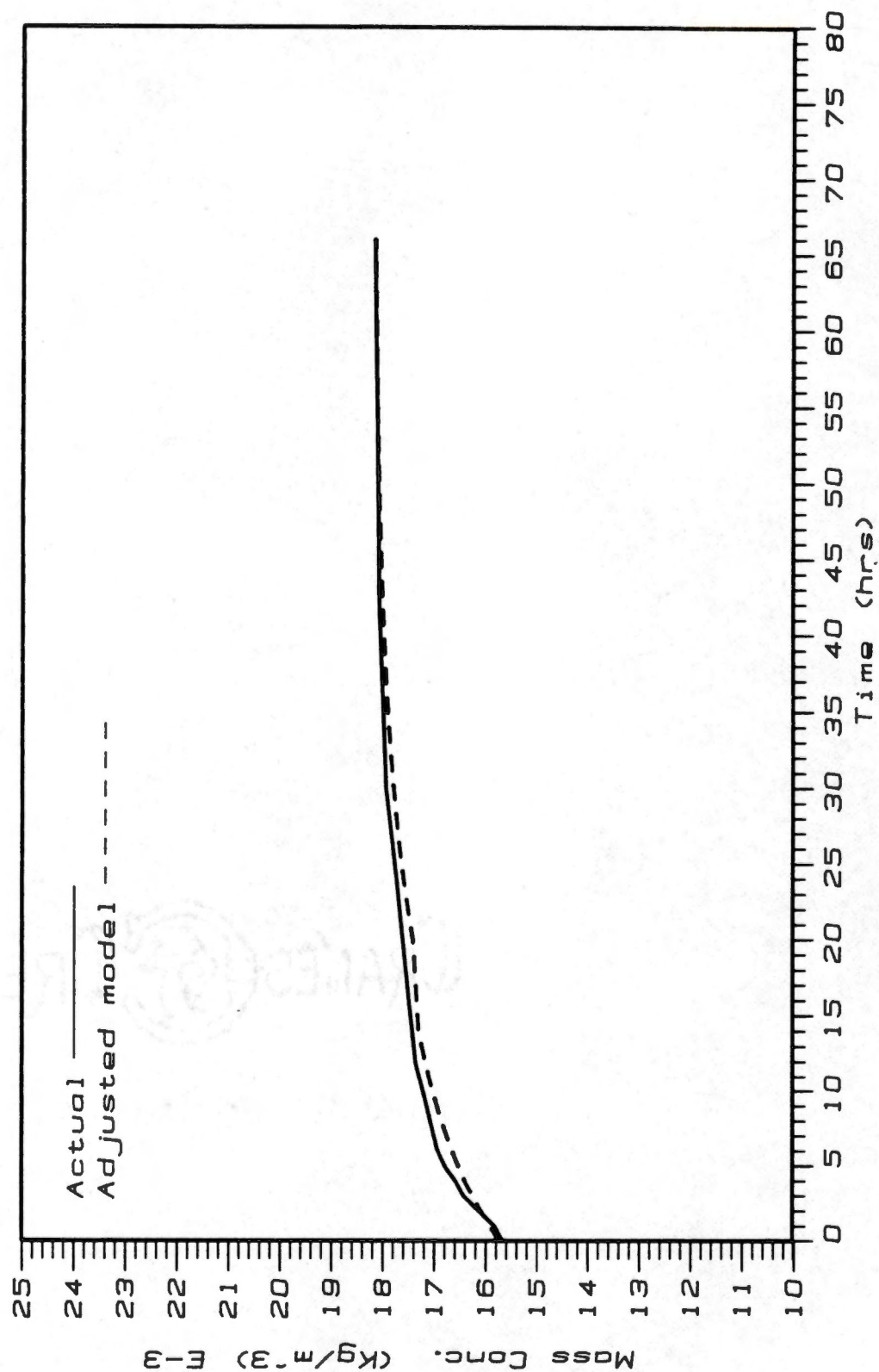


Figure 15. Comparison of Actual and Simulated Results with Model Adjusted to Remove Time Lag.

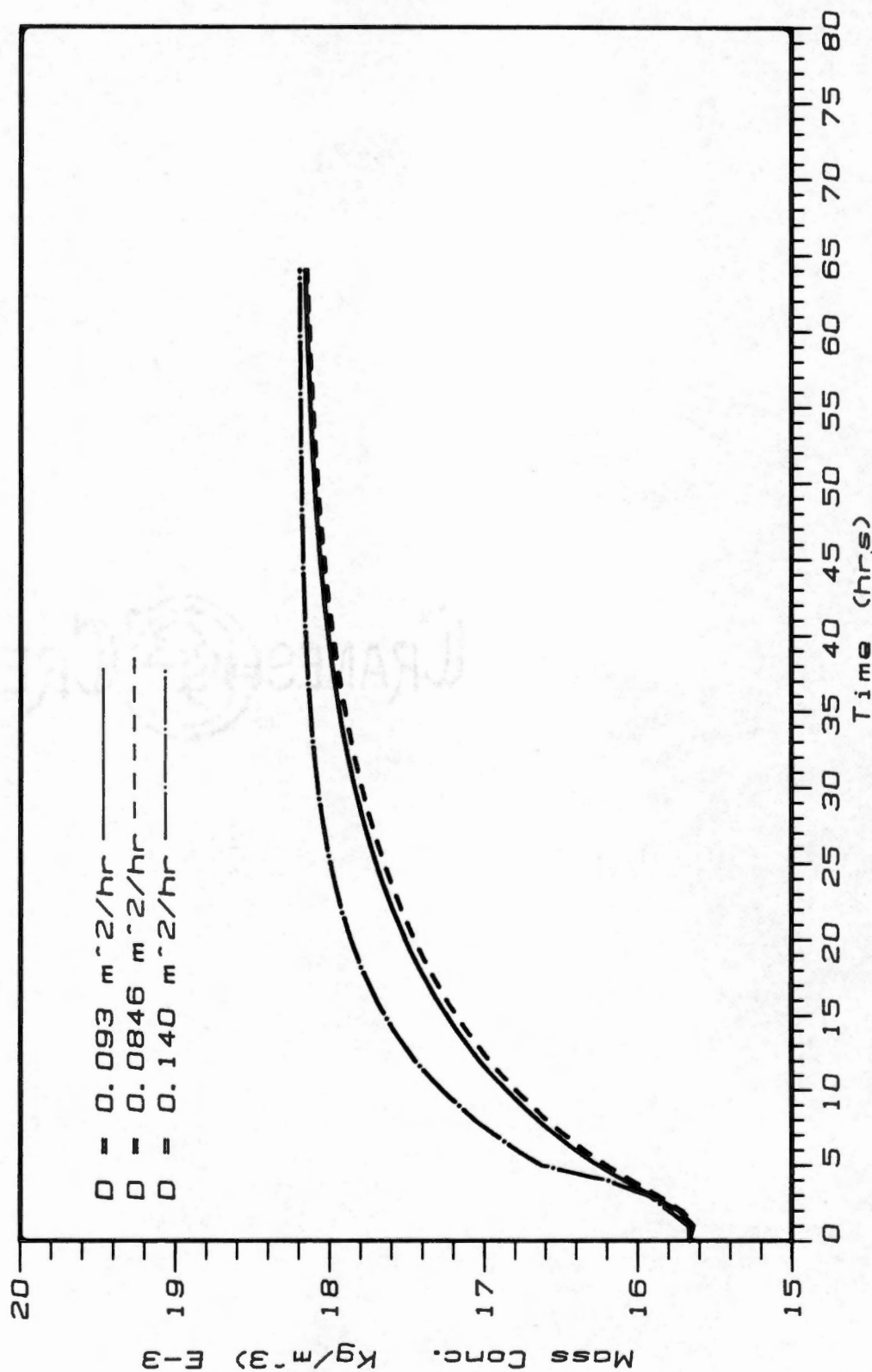


Figure 16. Sensitivity of the Rate of Change in Water Vapor Concentration to the Value of the Diffusion Coefficient.

Additional tests were performed in which the chamber was initially dehumidified to a low relative humidity, sealed, and allowed to reach equilibrium over a period of three days. A quantity of distilled water at approximately the chamber temperature was then introduced into a pan placed at the center of the chamber. Temperature and relative humidity data were then monitored for 72 hours. This amount of time was necessary to produce a chart of usable length due to the resolution of the hygrothermograph paper. Simulations were performed for this case by specifying the nodes occupied by the pan of water to be at saturation concentration for the water temperature. Examination of the results revealed that a fundamental difference existed between what was being modeled and what actually happened in the chamber. In the model, the saturation concentration specified at the center node implies that the moisture is already in vapor form. In the actual experiment, however, a phase change took place as liquid water in the pan evaporated. Thus the latent heat of vaporization was not accounted for in the simulation. The phase change was not intended to be modeled, and due to the fundamental differences which existed, no valid comparisons could be made between actual and simulated results for this experiment.

CHAPTER V

EXAMPLE OF A SPECIFIC APPLICATION

Nature of the Problem

The model was intentionally developed in a general form to allow flexibility in its application. An example of how the program can be modified for a specific application is presented in this chapter. It was desired to simulate the temperature and moisture response in an area in which a rotating sprinkler was operating. The expected effect of heat and mass transfer from the droplets in flight was a lowering of the temperature and an increase in the moisture content in the immediate vicinity. In order to model this problem, the generation subroutines for heat and mass had to be modified to account for transfer from the droplets. The time of rotation of the sprinkler was assumed to be one minute. Consequently, the generation was time-dependent. This fact complicated the analysis, however, with minor modifications the simulation was performed.

Interaction of Finite Element Grid with Droplet Trajectories

Simulation of the effects of heat and mass transfer from droplets in flight required the integration of droplet size distribution and trajectory data with the mechanisms of heat and mass transfer.

A distribution of droplet sizes is characteristic of irrigation sprinkler nozzles. Operating pressure and nozzle size are the primary system factors which affect this distribution. In order to accurately predict the amount of heat and mass transfer which occurs, the size distribution of droplets must be known. Chao (1969) found that the rate of heat and mass transfer from a droplet to the surrounding fluid is a function of the droplet radius to the three-halves power.

In addition to the droplet size distribution data, information about the trajectories of the droplets was necessary to obtain accurate results. Droplet size, operating pressure, and wind conditions are the primary factors which affect the path of flight. Trajectory data for droplet sizes between 0.2 mm and 6.0 mm in diameter were generated by a modified version of the SINLEG model developed by von Bernuth and Gilley (1984). This model uses a fourth order Runge-Kutta technique to solve the governing ballistics equations. Input conditions were 275.5 Kilopascals (kPa) operating pressure, with a 25 degree trajectory angle at the nozzle. Output included radial and vertical position coordinates, resultant velocities, and angles for each droplet size at 0.2 mm increments. Trajectories for droplets at 1.0 mm increments are shown in Figure 17. Resultant velocities of 1.0 mm size divisions are shown in Figure 18.

Curve Fitting

Curve fitting technique was applied to the trajectory data to obtain functional relationships between vertical and radial distance

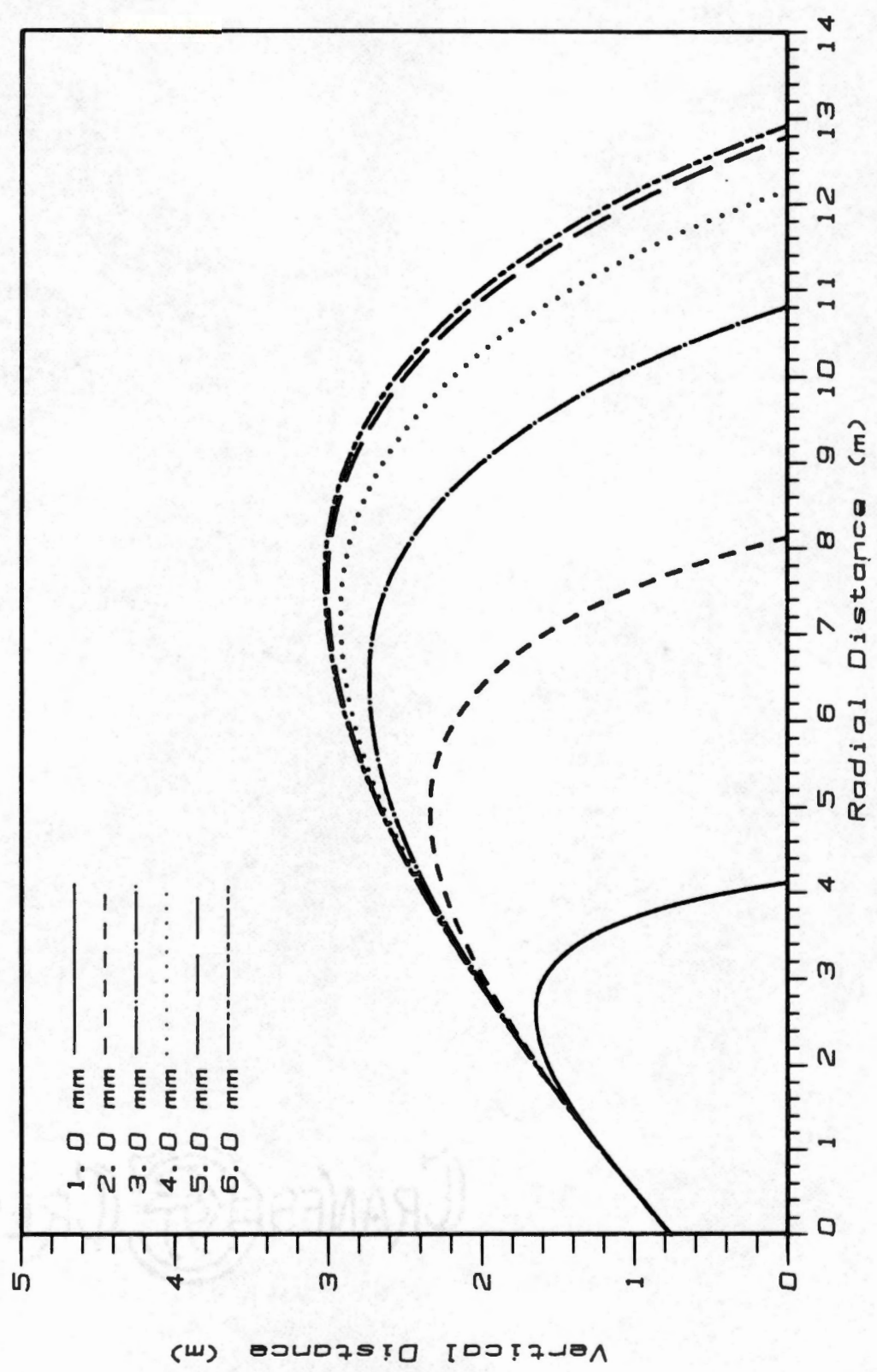


Figure 17. Trajectories for Selected Droplet Diameters.
(From von Bernuth and Gilley, 1984)

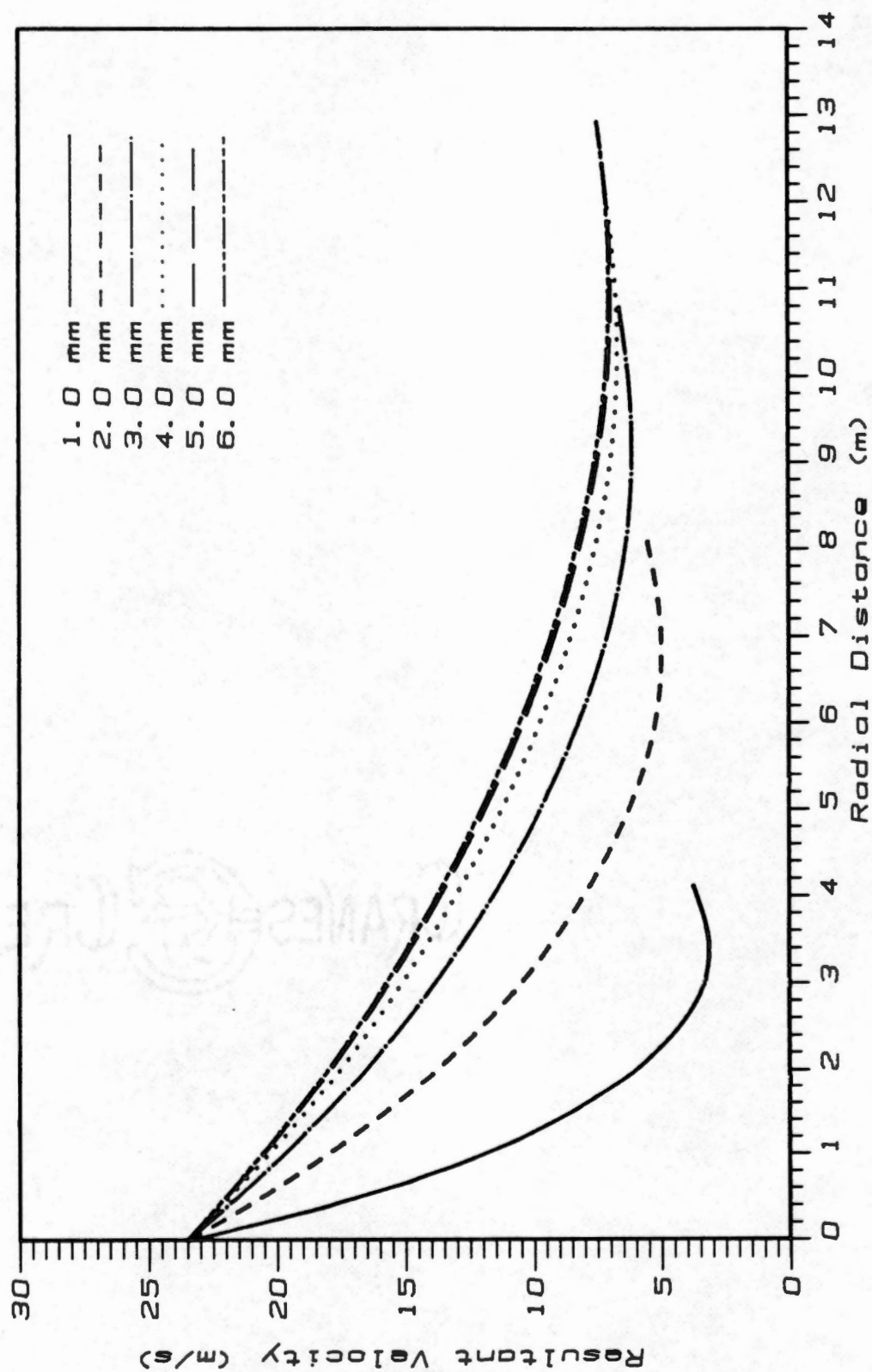


Figure 18. Resultant Velocities for Selected Droplet Diameters.
(From von Bernuth and Gilley, 1984)

as well as resultant velocity and radial distance. A fourth-order polynomial equation was found to be satisfactory for all droplet sizes larger than 0.8 mm. The remaining sizes could not be fitted adequately unless the data files were partitioned and fit in sections. The 0.2 mm droplet trajectory is nearly vertical after about 0.22 meter. A linear relationship was used for this section. Comparisons between fitted and actual position for two selected droplet sizes are shown in Figures 19 and 20.

Element/Trajectory Analysis

The trajectory and velocity information was used to route the droplets through a grid chosen for this problem. A FORTRAN program was written to determine the elements through which each droplet size would pass for the given conditions. In addition, the path length and average velocity were computed for each element. With this information the time that a droplet was in each element could be calculated. This was necessary in order to determine the amount of heat and mass transfer occurring within an element.

Droplet Transfer Equations

The transfer of heat and mass from a droplet in flight is a transient problem. Complications arise as a result of the high Reynolds number associated with droplets emitted from sprinkler nozzles. While numerous analyses have been performed for the case of small Reynolds number, very few solutions were available for the large Reynolds number case.

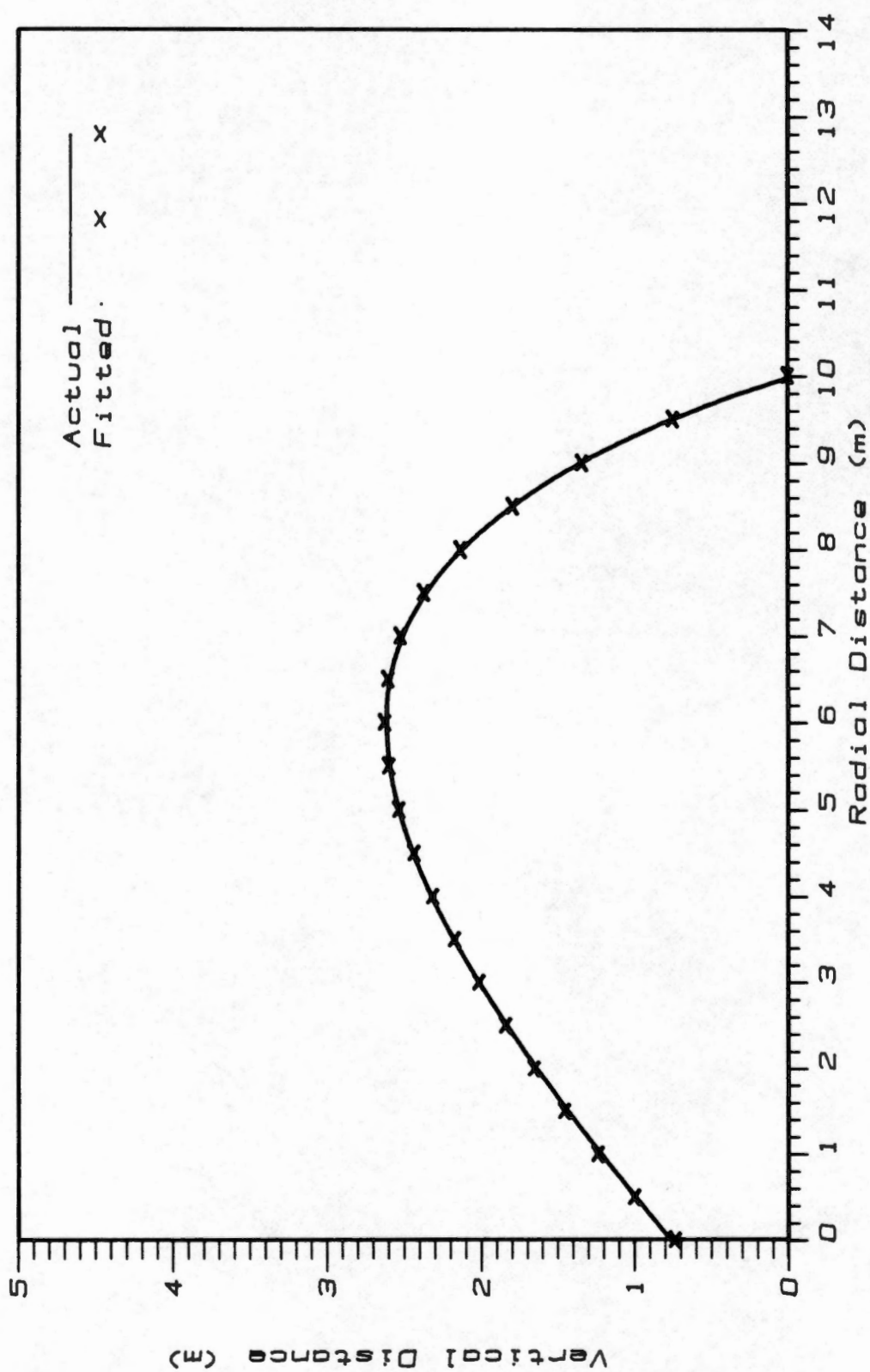


Figure 19. Comparison of Fitted and Actual Trajectories for a 2.6 mm Diameter Droplet.

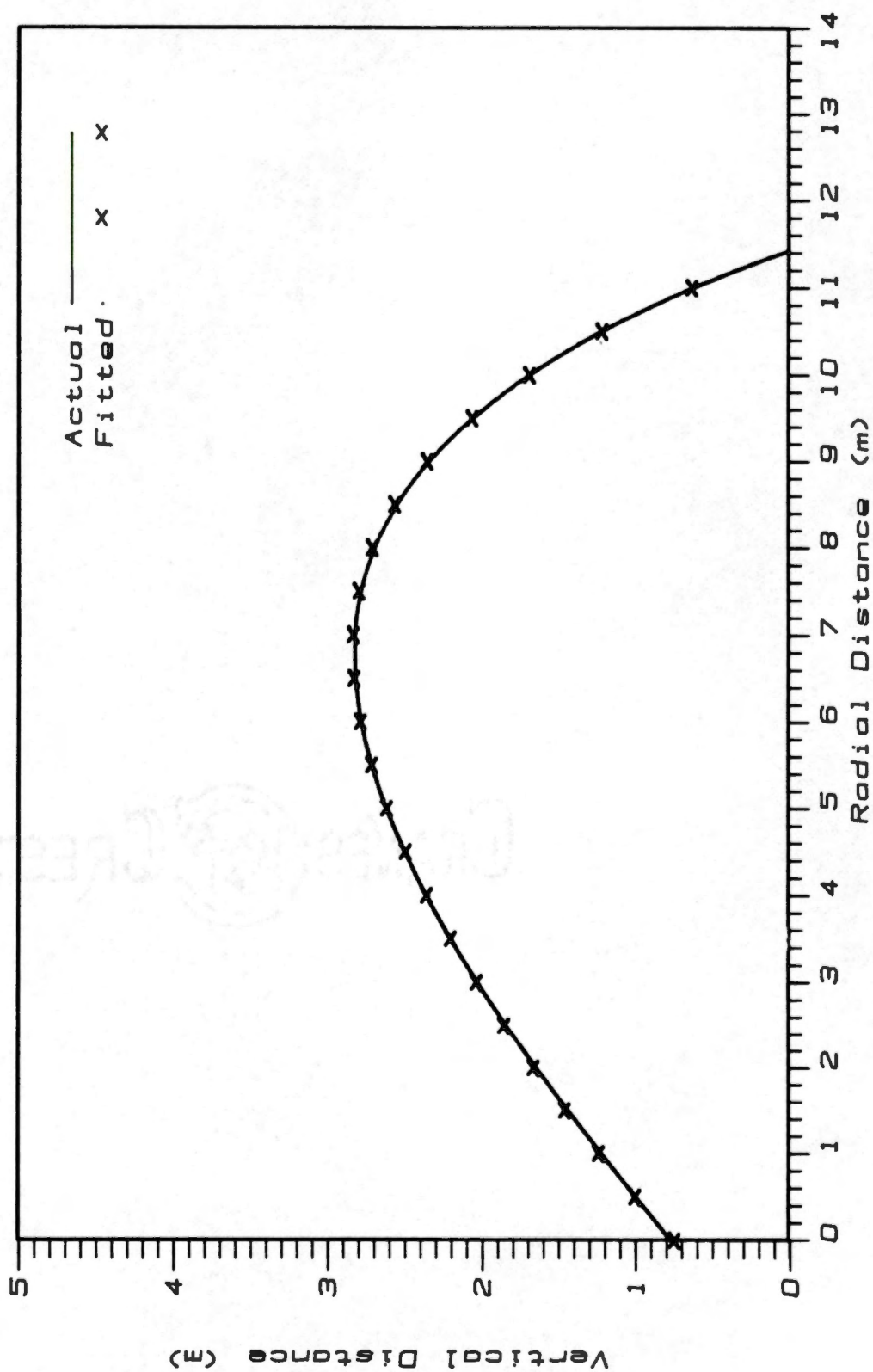


Figure 20. Comparison of Fitted and Actual Trajectories for a 3.4 mm Diameter Droplet.

Chao (1969), however, presented an enlightening analysis for the transient response behavior of a fluid sphere with internal circulation under conditions of high Reynolds and Peclet numbers. The similarities between Chao's problem statement and corresponding assumptions and the problem at hand were great. For this reason, Chao's equations for heat and mass transfer from droplets were adopted for use in the model. The choice of these equations was merely for convenience in illustrating the use of the user-supplied subroutines for a specific application.

For large Reynolds and Peclet numbers ($Pe = 2V_{avg}R/K_1$), the transient response behavior of the boundary layers was found to depend on a single dimensionless parameter, Ut/R , where: U is the velocity; t represents time; and R is the radius of the droplet (Chao, 1969). When this parameter equals one, the growth of the boundary layers is essentially complete. Considering a droplet with a radius of 2.0 mm traveling at 10 m/s, this means that the boundary layer growth is essentially complete after only 0.0002 second. The time of flight for a droplet of this size is about 1.5 seconds. This implies that an assumption of steady state conditions for heat and mass transfer would be reasonable. According to Chao's analysis, the total rate of heat transfer from the droplet to the outside fluid is:

$$Q = 2\pi R^2 \int_0^\pi q \sin \theta d\theta = \frac{4\sqrt{\pi} RK_1 (T_0 - T_\infty) Pe^{\frac{1}{2}}}{1 + \beta} I \quad (5-1)$$

where:

R = droplet radius

K = thermal conductivity

T_0 = initial droplet temperature

T_∞ = ambient temperature

$\beta = (K_1 c_1 \rho_1 / K_2 c_2 \rho_2)$

$Pe = 2V_{avg} R / k_1$

k = thermal diffusivity

$$I = \frac{\sqrt{3}}{4} \int_0^\pi \frac{\sin^3 \theta d\theta}{[(f - \cos \theta) - 1/3(f^3 - \cos^3 \theta)]^{1/2}}$$

$f = F(\theta, Pe, \text{time})$

1,2 = subscripts referring to exterior and interior of droplet respectively

For steady state conditions, I equals one and equation (5-1) reduces to:

$$Q = \frac{4\sqrt{\pi} \sqrt{2} K_1}{(1+\beta)k_1^{1/2}} R^{3/2} V_{avg}^{1/2} (t_0 - t_\infty) \quad (5-2)$$

The analogous mass transfer rate is written as follows:

$$M = \frac{4\sqrt{\pi} \sqrt{2} D_1^{1/2}}{(\alpha+\beta)} R^{3/2} V_{avg}^{1/2} (C_0 - \alpha C_\infty) \quad (5-3)$$

The total amount of heat or mass transfer within an element for a given droplet size would be equal to the product of the rate and the time of flight. Using the information obtained from the element/trajectory analysis, and knowing the droplet size distribution, the total amount of heat transfer could be determined for every element through which water passes. The total amount of heat or mass transfer was calculated using the average element temperature or concentration in equations (5-1) and (5-2).

Time-Dependent Generation

The equations for heat and mass transfer from the droplets were coded into the appropriate generation subroutines. The next step was to account for the intermittent nature of the presence of water due to sprinkler rotation. The time required for a complete revolution of the sprinkler was arbitrarily chosen to be one minute. For this reason, the integration steps (i.e., times at which the integration subroutine was called) were also chosen to be one minute. Considering only a single radius of rotation, water would be present for only a small portion of this time interval. Therefore, the integration subroutine needed to be modified to account for this time-dependent generation.

The IMSL Subroutine DVERK could not be modified. However, to use this subroutine, the user must supply an external subroutine in which the derivative expressions to be solved for are given. This subroutine was modified such that at the beginning of each new integration step, the generation subroutine was called and the influence

matrix was formed. Since DVERK uses a variable step method, the user has no control over the trial steps which are used in the numerical integration process. The easiest way to incorporate the time-dependent nature of the generation was to express the magnitude of generation as a mathematical function which could be built into the derivative expressions. A pulse function would be ideal since it is on for a finite period of time and off after the cutoff value. This function, however, is difficult to express mathematically, and was not practical for this problem. A negative exponential function is easily expressed and may be scaled such that it simulates a pulse. By equating the area under the negative exponential function with the total amount of heat or mass transfer within an element, this function could be used to represent the time-dependent generation.

Results and Discussion

The grid chosen for this problem contained 133 nodes and 216 elements (see Figure 21). The closest spacing was located in the vicinity of the sprinkler because all droplet sizes pass through this area. The outer boundaries of the region were assumed to be sufficiently far away that no temperature and concentration changes occurred at those nodes. Initial conditions (i.e., prior to sprinkling) were assumed to be 24.5 °C and 50 percent relative humidity at all nodes. Constant boundary conditions of 24.5 °C and 0.01133 Kg/m^3 (mass concentration at 24.5 °C and 50 percent relative humidity) were specified at the nodes along the top and side of the solution region. The

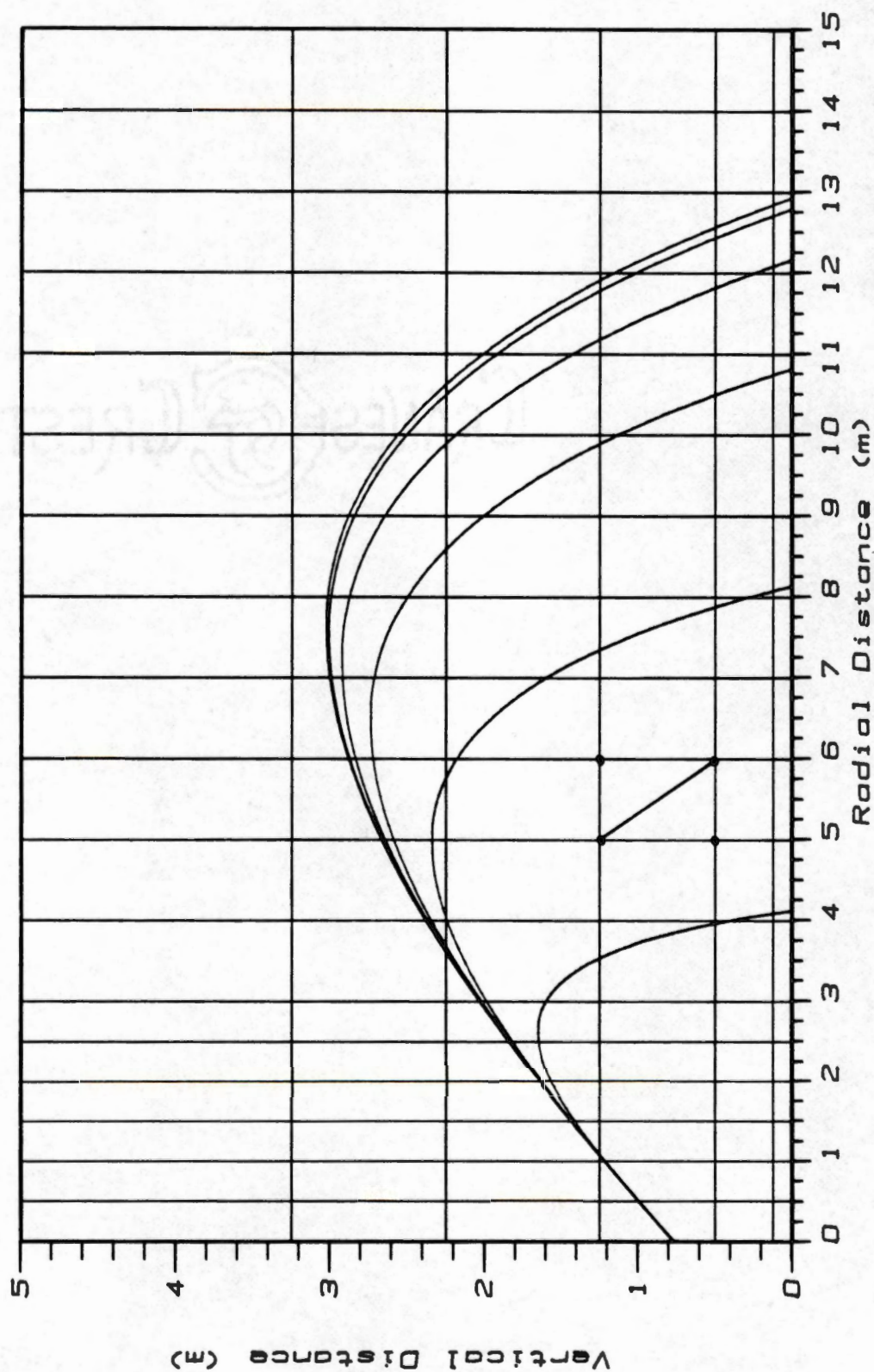


Figure 21. Grid Used in Droplet Simulations.

temperature at the lower boundary nodes was held constant at 24.5 °C, however, no concentrations were specified along this boundary. Under normal circumstances, the ground would be wet in the vicinity of the sprinkler. Evaporation from the ground is thought to be a significant portion of the total losses during sprinkling. In order to isolate the contribution of the droplets, it was necessary to assume that no evaporation occurred from the ground. The most efficient means of simulating this condition was to specify a mass flux of zero along this boundary. If no concentration is specified at a node, a flux of zero is automatically assigned to that node.

Two simulations were performed for two different water temperatures using the droplet size distribution shown in Table 2. In the first case, the water temperature was equal to the initial air temperature. Nodal values of temperature and concentration were obtained for a period of 6 hours. Variations in temperature were inconsequential, however, changes in concentration were significant.

The concentration at nodes 3 and 4 increased from the initial value of 0.01133 Kg/m³ to 0.023095 Kg/m³ and 0.023665 Kg/m³, respectively. These nodes lie immediately above and below the nozzle where the largest volume of water is concentrated (Figure 21). The saturation concentration for 24.5 °C is 0.01947 Kg/m³. This value represents the upper limit for mass transfer in vapor form. At this time, the saturation concentration is not accounted for in the model, so values larger than the saturated state are possible. If 0.01947 Kg/m³ were taken as the upper limit for this problem, the maximum increase in concentration at node 4 would be 71.9 percent rather than 108.9 percent.

Table 2. Droplet Size Distribution Used in Simulations.

Size (mm)	Frequency
0.2	324
0.4	330
0.6	421
0.8	390
1.0	362
1.2	227
1.4	148
1.6	83
1.8	66
2.0	40
2.2	35
2.4	15
2.6	19
2.8	13
3.0	6
3.2	7
3.4	6
3.6	2
3.8	2
4.0	1
4.2	3
4.4	1
4.6	1
4.8	0
5.0	0
5.2	0
5.4	1
5.6	0
5.8	0
6.0	0

The model showed that the increase in concentration was less significant as distance from the nozzle increased. This result is related to the ballistics and the size distribution of droplets. Given the same initial conditions (i.e., nozzle size, angle, and pressure), large droplets will travel farther than small droplets. Most irrigation sprinkler nozzles are characterized by a distribution of droplet sizes containing more small and intermediate sized droplets than large droplets. Thus, the greatest changes in temperature or concentration would be expected to occur near the sprinkler.

The second simulation represents the more realistic case in which the water temperature is lower than the ambient air temperature. Given this condition, an increase in the water vapor concentration and a decrease in temperature would be expected over time. The initial temperature and concentration were once again specified to be 24.5°C and 0.01133 Kg/m^3 , respectively. Water temperature was chosen to be 18.3°C and was assumed to remain constant. This is a simplification which is likely to introduce error, however, since the objective of this chapter was to illustrate the use of the model, this simplification seems reasonable. The general trends should still be valid.

Results for mass transfer were identical to those of the previous simulation. This is to be expected since the mass equation is independent of temperature. A slight temperature decrease was evident over the 6 hour period. The maximum depression was 3.1°C at node 4. The changes in concentration and temperature became less significant as distance from the sprinkler increased. A plot of the change in

temperature with time is shown for selected nodal positions in Figure 22. The results indicate that the equations used to determine heat and mass transfer from the droplets do not include the latent heat associated with evaporation of water. Consequently, the temperature changes only include effects of changes in sensible heat. In order to model the effects of evaporative cooling from droplets more realistically, the latent heat would need to be included. Additional cooling would be expected if the latent heat were incorporated into the model.

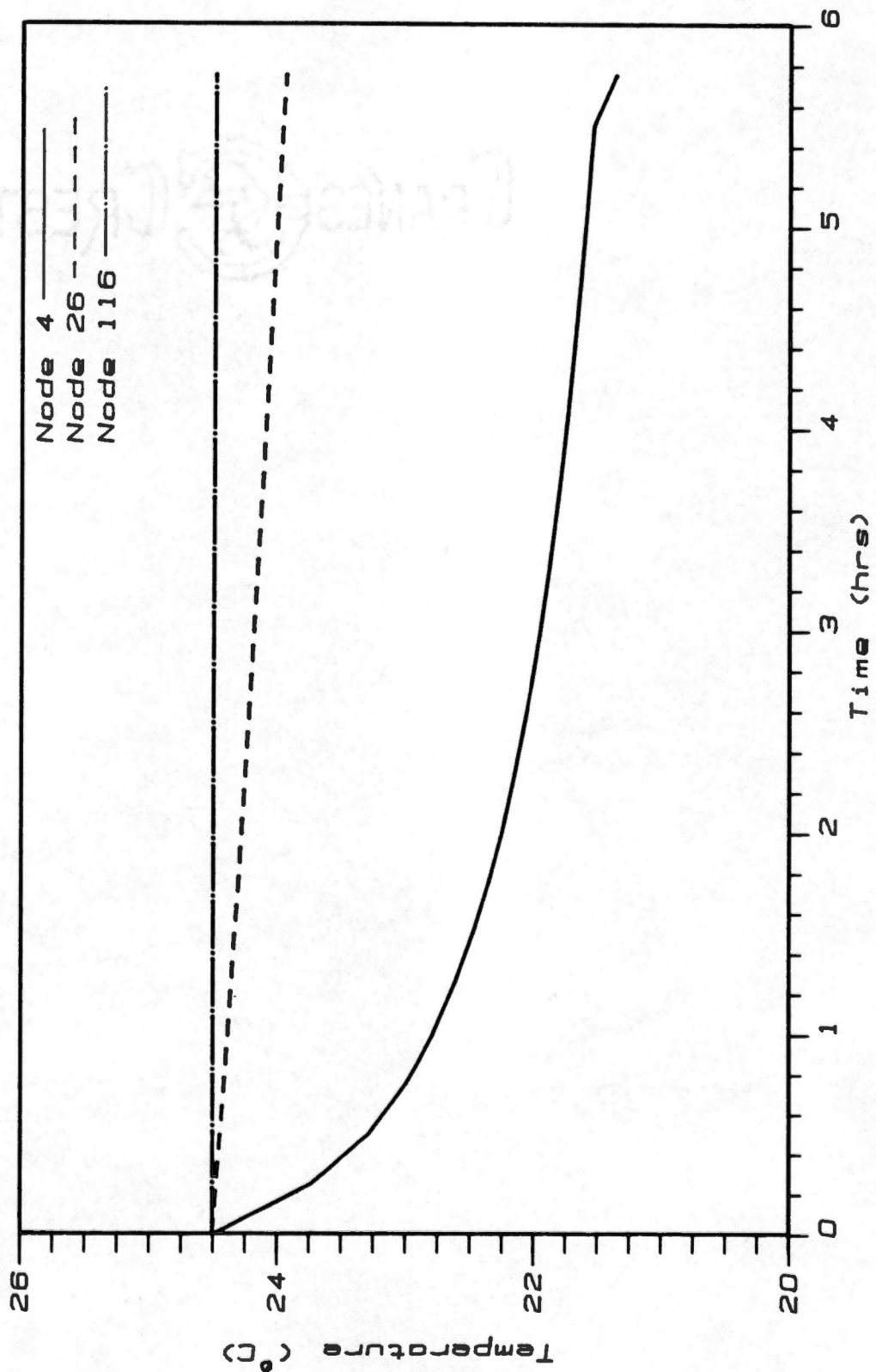


Figure 22. Plot of Temperature Change with Time for Selected Nodes.

CHAPTER VI

SUMMARY AND CONCLUSIONS

Summary

The operation of irrigation sprinklers may cause changes in the microclimate due to the effects of heat and mass transfer. A theoretical model which accounts for the diffusion of heat and mass in stagnant air was developed using equations for conservation of mass and energy. The geometry used in development of the governing equations was a two-dimensional radially axi-symmetric system. The finite element method was employed to solve the governing equations numerically. Element geometry was chosen to be a three-node linear triangle, and linear interpolation functions were used to approximate the value of the dependent variable in an element. Integration was performed by the IMSL subroutine DVERK which uses a variable order, variable step Runge-Kutta technique to solve a set of first order linear differential equations.

The model was developed in a general form to allow maximum flexibility in application. An example for adapting the program to a specific application by modifying the appropriate subroutines is given. The program was written in FORTRAN IV using the Fortran H extended enhanced compiler.

Since the mass equation was independent of temperature, the solution procedure was to solve for nodal concentrations during a given time interval and substitute the results into the energy equation to solve for nodal temperatures for the same interval. Accuracy of the coding and the theory was checked in two ways: comparison of model results with analytical solutions; and comparison of model results with experimental data.

Recommendations

Several improvements could be made which would increase the flexibility and accuracy of the model. The present method of solution places restrictions upon the size of the integration intervals. If the intervals are chosen to be large, error may become significant due to the assumption of constant nodal concentrations for the duration of the interval. A simultaneous solution of both conservation equations would be desirable, however, this was not feasible for the triangular element geometry and linear interpolation functions due to memory and execution time requirements. The use of a higher order element such as a six node triangle or a general quadrilateral along with a higher order approximating function would increase the accuracy of the solution and consequently reduce the number of nodes required.

Another improvement would be the provision to compare nodal concentrations with the saturation concentration at the current nodal temperature. This would provide a means of determining when and where condensation occurs within the solution region. Equations for

saturation concentration as a function of temperature are available which could be coded into the appropriate subroutines and used to check values after each integration. Alternatively, actual values could be interpolated from a data file in order to reduce the number of computations. This process would increase execution time since comparisons would probably be made after every integration, but the value of the results may justify the reduction in speed.

Perhaps the most useful addition to the model would be the ability to account for the effects of phase changes explicitly. Modification of the microclimate involves changes in both sensible and latent heat. If the model is to be used to simulate these kinds of problems, provision should be made to include all pertinent energy terms. Possible applications include evaporative cooling and frost protection. In addition, the effects of external factors such as wind and radiation would be desirable.

Conclusions

A major objective of this research was to maintain generality in the development of a theory which would contribute to the understanding of complex phenomena accompanying the operation of irrigation sprinklers. While the present model may appear to possess deficiencies, the suggested improvements would be of little value without the general provision to account for the diffusion of the respective heat or mass. In this sense, the objectives have been met. The close agreement between simulated results and both analytical solutions and

experimental data indicates that the development of the theory is correct. Simulations of actual conditions of sprinkling showed the expected trends of temperature decrease and moisture content increase. Additional testing and refinements should be made, and improvements should be incorporated as the need arises. This work should be interpreted as an initial step toward a better understanding of the complex interactions between heat and mass transfer and their effects upon the local environment. The next step in the research process is to evaluate the information obtained in order to build upon the results.



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APPENDIXES



APPENDIX A
MATRIX NOTATION

SUMMARY OF MATRIX NOTATION FOR MASS EQUATION

$$\frac{\pi \bar{r} D}{2A} \begin{bmatrix} b_i b_i + c_i c_i & b_i b_j + c_i c_j & b_i b_k + c_i c_k \\ b_i b_j + c_i c_j & b_j b_j + c_j c_j & b_j b_k + c_j c_k \\ b_i b_k + c_i c_k & b_j b_k + c_j c_k & b_k b_k + c_k c_k \end{bmatrix} \begin{Bmatrix} \rho_i \\ \rho_j \\ \rho_k \end{Bmatrix} \quad \text{CME}$$

$$\frac{\pi \rho_a c_a A}{30} \begin{bmatrix} 4r_i + 6\bar{r} & r_i + r_j + 3\bar{r} & r_i + r_k + 3\bar{r} \\ r_i + r_j + 3\bar{r} & 4r_j + 6\bar{r} & r_j + r_k + 3\bar{r} \\ r_i + r_k + 3\bar{r} & r_j + r_k + 3\bar{r} & 4r_k + 6\bar{r} \end{bmatrix} \begin{Bmatrix} \dot{\rho}_i \\ \dot{\rho}_j \\ \dot{\rho}_k \end{Bmatrix} \quad \text{STME}$$

$$\frac{\pi W' A}{2} \begin{Bmatrix} r_i/3 + \bar{r} \\ r_j/3 + \bar{r} \\ r_k/3 + \bar{r} \end{Bmatrix} \quad \text{MGME}$$

Element equations in matrix form:

$$[\text{STME}] \{\dot{\rho}\} + [\text{CME}] = \{\text{MGME}\} - \{\text{RHS}\}$$

SUMMARY OF MATRIX NOTATION FOR ENERGY EQUATION

$$\frac{\pi \rho_a c_a A}{30} \begin{bmatrix} 4r_i + 6\bar{r} & r_i + r_j + 3\bar{r} & r_i + r_k + 3\bar{r} \\ r_i + r_j + 3\bar{r} & 4r_j + 6\bar{r} & r_j + r_k + 3\bar{r} \\ r_i + r_k + 3\bar{r} & r_j + r_k + 3\bar{r} & 4r_k + 6\bar{r} \end{bmatrix} \begin{Bmatrix} \dot{T}_i \\ \dot{T}_j \\ \dot{T}_k \end{Bmatrix} \quad \text{STTE1}$$

$$\frac{\pi c_w A}{90} \left(\rho_i \begin{bmatrix} 9r_i + 9\bar{r} & 2r_i + r_j + 3\bar{r} & 2r_i + r_k + 3\bar{r} \\ 2r_i + r_j + 3\bar{r} & r_i + 2r_j + 3\bar{r} & 3\bar{r} \\ 2r_i + r_k + 3\bar{r} & 3\bar{r} & r_i + 2r_k + 3\bar{r} \end{bmatrix} + \right.$$

$$\rho_j \begin{bmatrix} 2r_i + r_j + 3\bar{r} & r_i + 2r_j + 3\bar{r} & 3\bar{r} \\ r_i + 2r_j + 3\bar{r} & 9r_j + 9\bar{r} & 2r_i + r_k + 3\bar{r} \\ 3\bar{r} & 2r_j + r_k + 3\bar{r} & r_j + 2r_k + 3\bar{r} \end{bmatrix} +$$

$$\rho_k \begin{bmatrix} 2r_i + r_k + 3\bar{r} & 3\bar{r} & r_i + 2r_k + 3\bar{r} \\ 3\bar{r} & 2r_j + r_k + 3\bar{r} & r_j + 2r_k + 3\bar{r} \\ r_i + 2r_k + 3\bar{r} & r_j + 2r_k + 3\bar{r} & 9r_k + 9\bar{r} \end{bmatrix} \begin{Bmatrix} \dot{T}_i \\ \dot{T}_j \\ \dot{T}_k \end{Bmatrix} \quad \text{STTE2}$$

$$\frac{\pi \bar{r} K}{2A} \begin{bmatrix} b_i b_i + b_i b_j & c_i c_j + c_i c_k & b_i b_k + c_i c_k \\ b_i b_j + c_i c_j & b_j b_j + c_j c_j & b_j b_k + c_j c_k \\ b_i b_k + c_i c_k & b_j b_k + c_j c_k & b_k b_k + c_k c_k \end{bmatrix} \begin{Bmatrix} T_i \\ T_j \\ T_k \end{Bmatrix} \quad \text{TME1}$$

$$\frac{\pi D_c w}{24A} [b_i b_j b_k] \begin{Bmatrix} \rho_i \\ \rho_j \\ \rho_k \end{Bmatrix} \begin{bmatrix} b_i(r_i + 3\bar{r}) & b_j(r_i + 3\bar{r}) & b_k(r_i + 3\bar{r}) \\ b_i(r_j + 3\bar{r}) & b_j(r_j + 3\bar{r}) & b_k(r_j + 3\bar{r}) \\ b_i(r_k + 3\bar{r}) & b_j(r_k + 3\bar{r}) & b_k(r_k + 3\bar{r}) \end{bmatrix} \begin{Bmatrix} T_i \\ T_j \\ T_k \end{Bmatrix} \quad \text{TME2}$$

$$\frac{\pi D_c w}{24A} [c_i c_j c_k] \begin{Bmatrix} \rho_i \\ \rho_j \\ \rho_k \end{Bmatrix} \begin{bmatrix} c_i(r_i + 3\bar{r}) & c_j(r_i + 3\bar{r}) & c_k(r_i + 3\bar{r}) \\ c_i(r_j + 3\bar{r}) & c_j(r_j + 3\bar{r}) & c_k(r_j + 3\bar{r}) \\ c_i(r_k + 3\bar{r}) & c_j(r_k + 3\bar{r}) & c_k(r_k + 3\bar{r}) \end{bmatrix} \begin{Bmatrix} T_i \\ T_j \\ T_k \end{Bmatrix} \quad \text{TME3}$$

$$\frac{\pi g''' A}{2} \begin{Bmatrix} r_i/3 + \bar{r} \\ r_j/3 + \bar{r} \\ r_k/3 + \bar{r} \end{Bmatrix} \quad \text{QGME}$$

Grouping like terms:

$$[STTE] = [STTE1] + [STTE2]$$

$$[TME] = [TME1] + [TME2] + [TME3]$$

Element equations in matrix form:

$$[STTE] \{\dot{T}\} + [TME] \{T\} = \{QGME\} - \{RHS\}$$

APPENDIX B
IMSL SUBROUTINES

IMSL SUBROUTINES

- DVERK - Integration subroutine which solves a set of simultaneous first order linear differential equations using a variable order, variable step Runge-Kutta technique.
- FCN - User-supplied subroutine containing the expressions for the derivatives to be solved by DVERK.
- LINV2F - Subroutine for matrix inversion.
- VMULFF - Subroutine for matrix multiplication.
- VMULFM - Subroutine for multiplying the transpose of a matrix by another matrix.
- EIGRF - Subroutine for determining the eigenvalues and eigenvectors of a matrix.

APPENDIX C
PROGRAM LISTING

```

C*****
C*
C*          TRANSFER FORTRAN
C*
C*          JOEL G. HALL
C*
C*****
C
C  PROGRAM DESCRIPTION:
C
C    THIS PROGRAM USES A FINITE ELEMENT ANALYSIS TO SIMULATE THE
C    SIMULTANEOUS DIFFUSION OF HEAT AND MASS THROUGH STAGNANT AIR.
C    THE GOVERNING EQUATIONS INCLUDE CONSERVATION OF MASS AND
C    CONSERVATION OF ENERGY. THE FOLLOWING ASSUMPTIONS WERE MADE
C    IN THE DEVELOPMENT OF THE GOVERNING EQUATIONS:
C
C      1.  CONSTANT TRANSFER COEFFICIENTS,
C      2.  NO PRESSURE DIFFUSION,
C      3.  NO THERMAL DIFFUSION (SORET EFFECT),
C      4.  EFFECT OF GRAVITY NEGLECTED,
C      5.  HEAT TRANSFER BY CONDUCTION ONLY,
C      6.  STAGNANT AIR, AND
C      8.  RADially AXISYMMETRIC GEOMETRY.
C
C
C    THE MASS EQUATION IS INDEPENDENT OF THE ENERGY EQUATION, HOW-
C    EVER THE ENERGY EQUATION IS COUPLED DUE TO THE FACT THAT ENERGY
C    TRANSFER ACCOMPANIES MASS TRANSFER. THE METHOD OF SOLUTION
C    INVOLVES SOLVING THE MASS EQUATION FOR NODAL CONCENTRATIONS
C    AT A GIVEN TIME STEP AND SUBSTITUTING THESE VALUES INTO
C    THE ENERGY EQUATION TO SOLVE FOR NODAL TEMPERATURES AT THE
C    SAME TIME STEP.  THUS THE TWO EQUATIONS ARE SOLVED SEPERATELY.
C    THIS PROCEDURE ASSUMES THAT THE MASS REMAINS CONSTANT DURING
C    THE TIME STEP.  CHOICE OF APPROPRIATE TIME STEPS IS THEREFORE
C    RELATED TO THE ACCURACY OF THE SOLUTION.
C
C*****
C
C    DIMENSION ARRAYS AND DECLARE VARIABLES
C
C    178x178 IS THE BIGGEST ALLOWABLE ARRAY SIZE
C
C*****
C*****
C
C    NOTE:  THESE ARRAYS MUST BE DIMENSIONED EXACTLY TO THE
C           NUMBER OF NODES USED IN THE GRID.
C
C
C    DOUBLE PRECISION STML(63,63),STMINV(63,63),CMA(63,63),T(63)
C    DOUBLE PRECISION CEVEC(63,63),CEINV(63,63),STTL(63,63),CNC(63)
C    DOUBLE PRECISION TML(63,63),CETKE(63,63),CINIT(63)
C    DOUBLE PRECISION STLINV(63,63),TMA(63,63),TEVEC(63,63)
C    DOUBLE PRECISION TEINV(63,63),CETG(63),CETCE(63,63)

```

```

DOUBLE PRECISION CPRIME(63),CN(63),TETG(63),TETCE(63,63)
DOUBLE PRECISION TETKE(63,63),TPRIME(63),TN(63),CML(63,63)
DOUBLE PRECISION F(63),G(63),RHST(63),RHSL(63),QGML(63)
DOUBLE PRECISION CETC(63,63),TETC(63,63),TINIT(63)
REAL*8 MGML(63)
COMPLEX*16 CEVECC(63,63),CEVAL(63),TEVECC(63,63),TEVAL(63)

```

```

C
C*****
C

```

```

DOUBLE PRECISION STTM(63,63),CMM(63,63),TM(63,63)
DOUBLE PRECISION STMM(63,63),WKAREA(12000),TOL
DOUBLE PRECISION TME1(3,3),TME2(3,3),SITE1(3,3),TME3(3,3),C(24)
DOUBLE PRECISION TME(3,3),STME(3,3),CME(3,3),STTE2(3,3),STTE(3,3)
DOUBLE PRECISION XC(63),YC(63),RBAR(80),DEL(80)
DOUBLE PRECISION XCE(3),YCE(3),B(80,3),CH(80,3)
DOUBLE PRECISION Q(80),W(63,9)
DOUBLE PRECISION QGM(80),CNCE(3),CGME(3),QG(80)
DOUBLE PRECISION TT,TTEND,CUTOFF,TSTEP,TSTEP2,TSTRT,TSTRT2,ENTM
DOUBLE PRECISION A1,A2,A3,B1,B2,B3,C1,C2,C3,ZBAR
DOUBLE PRECISION CONST,RHOA,CP,CA,P1,TNT,TO,CNCO,TK(80),D(80)
REAL*8 MGME(3),MGML(63),MG(80),PSTEP(50),NNCNC
INTEGER NUDE(80,3),NN,NE,N,NGEN
INTEGER CNS(63),NQSC(63),NTS(63),NQST(63)
INTEGER NNSC,NQ,NWSQC,NCNC,NH,IND,IER,IDGT,NT,NNST
INTEGER GFLAG,NWSQT,KQC,KQT
EXTERNAL FCN1,FCN2
COMMON /TEMP/ TETCE,TETKE,TETG,G,TSTRT2
COMMON /CUNC/ CETCE,CETKE,CETG,F,TSTRT
COMMON /GEN/ CEVEC,TEVEC,REAR,DEL,XC,NCSC,NQST,NWSQC,NWSQT,NN,NE
*,NODE,IER

```

```

C
C      READ THE NUMBER OF SYSTEM NODES AND ELEMENTS
C

```

```

      READ(21,*) NN,NE
      WRITE(23,1035) NN,NE
      WRITE(22,3450)

```

```

C
C      INITIALIZE PARAMETERS
C

```

```

8      TSTRT=0.
      DO 4 I=1,50
      PSTEP(I)=0.
4      CONTINUE
      NMAX=NN
      GFLAG=0
      CFLAG=0
      NWSQC=0
      NWSQT=0
      NNST=0
      NNSC=0
      DO 9 I=1,NN
      RHSL(I)=0.
      RHST(I)=0.
      CNC(I)=0.
      T(I)=0.

```



```

CINIT(I)=0.
TINIT(I)=0.
CPRIME(I)=0.
TPRIME(I)=0.
MGM(J)=0.
QGM(J)=0.
UGML(I)=0.
MGML(I)=0.
NQSC(I)=0
NQST(I)=0
NTS(I)=0
CNS(I)=0
Q(I)=0.
CEVAL(I)=0.
TEVAL(I)=0.
CN(I)=0.
TN(I)=0.
F(I)=0.
G(I)=0.
CETG(I)=0.
TETG(I)=0.
XC(I)=0.
YC(I)=0.
DO 9 J=1,N
CMM(I,J)=0.
TM(I,J)=0.
CMA(I,J)=0.
TMA(I,J)=0.
CML(I,J)=0.
STMM(I,J)=0.
STTM(I,J)=0.
STMINV(I,J)=0.
STLINV(I,J)=0.
STML(I,J)=0.
STTL(I,J)=0.
TML(I,J)=0.
CEVECC(I,J)=0.
TEVECC(I,J)=0.
CEVEC(I,J)=0.
TEVEC(I,J)=0.
CETC(I,J)=0.
TETC(I,J)=0.
CETCE(I,J)=0.
TETCE(I,J)=0.
CETKE(I,J)=0.
TETKE(I,J)=0.
CEINV(I,J)=0.
TEINV(I,J)=0.
CONTINUE
DO 10 I=1,3
XCE(I)=0.
YCE(I)=0.
MGME(I)=0.
UGME(I)=0.
CNCE(I)=0.

```

```

DO 11 M=1,3
CME(1,M)=0.
TME(1,M)=0.
TME1(1,M)=0.
TME2(1,M)=0.
TME3(1,M)=0.
STME(1,M)=0.
STTE1(1,M)=0.
STTE2(1,M)=0.
STTE(1,M)=0.
11 CONTINUE
DO 10 J=1,NE
B(J,1)=0.
CH(J,1)=0.
DEL(J)=0.
D(J)=0.
TK(J)=0.
RBAR(J)=0.
NUDE(J,1)=0.
MG(J)=0.
OG(J)=0.
10 CONTINUE
C
C READ NODE NUMBERS AND NODAL COORDINATES
C
DO 15 I=1,NN
15 READ(21,*) J,XC(J),YC(J)
WRITE(23,1040)
DO 20 I=1,NN
20 WRITE(23,1045) I,XC(I),YC(I)
C
C READ SYSTEM TOPOLOGY (ELEMENT NO. AND NODE NUMBERS
C IN COUNTER-CLOCKWISE FASHION STARTING AT ANY NODE)
C
DO 30 I=1,NE
30 READ(21,*) J,NODE(J,1),NODE(J,2),NODE(J,3)
WRITE(23,1050)
DO 40 I=1,NE
40 WRITE(23,1055) I,NODE(I,1),NODE(I,2),NODE(I,3)
C
C READ INITIAL NODAL TEMPERATURES AND CONCENTRATIONS
C
BE3=0.
WRITE(23,1036)
READ(21,*) CNC0,TO
WRITE(23,1037) CNC0,TO
DO 90 I=1,NN
T(I)=TO
CNC(I)=CNC0
WRITE(22,3500) BE3,I,CNC(I),T(I)
90 CONTINUE
C
C THE FOLLOWING SECTIONS DEAL WITH BOUNDARY CONDITIONS WHICH ARE TO
C BE ENFORCED DURING THE SOLUTION. TWO KINDS OF BOUNDARY CONDITIONS
C MAY BE USED: SPECIFIED TEMPERATURE, AND SPECIFIED CONCENTRATION.

```

```

C   IF NEITHER IS SPECIFIED, A FLUX OF ZERO IS ASSIGNED TO THAT NODE.
C
C   READ SPECIFIED TEMPERATURES AND NODE NUMBERS INTO A LIST
C
      WRITE(23,1061)
      DO 55 I=1,NN
      READ(21,*) NT,TNT
      IF(NT.EQ.0) GO TO 65
      NTS(I)=NT
      T(NTS(I))=TNT
      WRITE(23,1062) I,NTS(I),T(NTS(I))
55    CONTINUE
C
C   COUNT NODES WITH SPECIFIED TEMPERATURE
C
65    NNST=I-1
C
C   READ SPECIFIED CONCENTRATIONS AND NODE NUMBERS INTO A LIST
C
      WRITE(23,1060)
      DO 50 I=1,NN
      READ(21,*) NCNC,NNCNC
      IF(NCNC.EQ.0) GO TO 60
      CNS(I)=NCNC
      CNC(CNS(I))=NNCNC
      WRITE(23,1065) I,CNS(I),CNC(CNS(I))
50    CONTINUE
C
C   COUNT NODES HAVING SPECIFIED CONCENTRATION
C
60    NNSC=I-1
C
C   SPECIFY EXTERNAL FLUX AND CORRESPONDING NODES FOR CONCENTRATION
C
      WRITE(23,1080)
      KQC=0
      DO 70 I=1,NN
      DO 68 J=1,NN
68    IF(1.EQ.CNS(J)) GO TO 70
      KQC=KQC+1
      NSQC(KQC)=I
      Q(I)=0.
      WRITE(23,1085) KQC,I,Q(I)
70    CONTINUE
      NNSQC=KQC
C
C   SPECIFY EXTERNAL FLUX AND CORRESPONDING NODES FOR ENERGY
C
      WRITE(23,1081)
      KQT=0
      DO 71 I=1,NN
      DO 69 J=1,NN
69    IF(1.EQ.NTS(J)) GO TO 71
      KQT=KQT+1
      NOST(KQT)=I

```



```

      Q(I)=0.
      WRITE(23,1085) KQT,1,Q(I)
71    CONTINUE
      NWSQT=KQT
C
C    READ THERMAL CONDUCTIVITY FOR EACH ELEMENT
C
      WRITE(23,1070)
      DO 75 I=1,NE
      READ(21,*) J,TK(J)
      WRITE(23,*) J,TK(J)
75    CONTINUE
C
C    READ DIFFUSION COEFFICIENT FOR EACH ELEMENT
C
      WRITE(23,1071)
      DO 80 I=1,NE
      READ(21,*) J,D(J)
      WRITE(23,*) J,D(J)
80    CONTINUE
C
C    READ AIR AND WATER VAPOR PROPERTIES (DENSITIES,SPECIFIC HEATS)
C
      WRITE(23,1072)
      READ(21,*) RHCA,CP,CA
      WRITE(23,1073) RHCA,CP,CA
C
C    READ IN INFORMATION FOR PARTITIONING THE INTEGRATION STEPS. ENTM
C    IS THE ENDING TIME FOR THE PROBLEM. CUTOFF IS THE VALUE OF TIME
C    WHICH PARTITIONS THE PROBLEM INTO TWO INTERVALS - FOR VALUES OF
C    TIME LESS THAN THE SPECIFIED CUTOFF, A SMALL TIME STEP (TSTEP1) IS
C    USED; FOR TIMES AFTER THE CUTOFF, A LARGER TIME STEP (TSTEP2) IS
C    USED. THIS ONLY REFERS TO TIMES WHEN THE INTEGRATION SUBROUTINE
C    IS CALLED - THE USER HAS NO CONTROL OVER THE TIME STEPS THAT THE
C    INTEGRATION SUBROUTINE USES.
C
      READ(21,*) ENTM,CUTOFF,TSTEP,TSTEP2
      WRITE(23,1077)
      WRITE(23,1074) ENTM,CUTOFF,TSTEP,TSTEP2
      TTEND=TTSTEP
C
C    READ IN THE NUMBER OF PRINT STEPS AND THE DESIRED TIMES
C    NOTE: THE VALUE OF TIME FOR WHICH OUTPUT IS DESIRED MUST
C    COINCIDE WITH A VALUE OF TIME FOR WHICH AN INTEGRATION
C    WAS PERFORMED.
C
      READ (21,*) NPRT
      WRITE(23,1075)
      DO 85 I=1,NPRT
      READ(21,*) PSTEP(I)
      WRITE(23,1076) I,PSSTEP(I)
85    CONTINUE
C
C    CYCLE FOR EACH ELEMENT AND FORM SYSTEM MATRICES
C    WHICH ARE CONSTANT (ONE-TIME CALCULATIONS)

```

```

C
C
C
C
      DO 140 K=1,NE
      K IS NOW THE ELEMENT NUMBER

      XCE(1)=XC(NODE(K,1))
      XCE(2)=XC(NODE(K,2))
      XCE(3)=XC(NODE(K,3))
      YCE(1)=YC(NODE(K,1))
      YCE(2)=YC(NODE(K,2))
      YCE(3)=YC(NODE(K,3))
      ZBAR=(YCE(1)+YCE(2)+YCE(3))/3.
      KBAR(K)=(XCE(1)+XCE(2)+XCE(3))/3.
      A1=XCE(2)*YCE(3)-XCE(3)*YCE(2)
      A2=XCE(3)*YCE(1)-XCE(1)*YCE(3)
      A3=XCE(1)*YCE(2)-XCE(2)*YCE(1)
      B(K,1)=YCE(2)-YCE(3)
      B(K,2)=YCE(3)-YCE(1)
      B(K,3)=YCE(1)-YCE(2)
      CH(K,1)=XCE(3)-XCE(2)
      CH(K,2)=XCE(1)-XCE(3)
      CH(K,3)=XCE(2)-XCE(1)
      DEL(K)=0.5*DAABS((XCE(1)*(YCE(2)-YCE(3))+
      *XCE(2)*(YCE(3)-YCE(1))+
      *XCE(3)*(YCE(1)-YCE(2))))
      PI=3.1415927

C
C
C
      FORM INFLUENCE MATRIX FOR CONCENTRATION

      B1=B(K,1)
      B2=B(K,2)
      B3=B(K,3)
      C1=CH(K,1)
      C2=CH(K,2)
      C3=CH(K,3)
      CONST=(2.*PI*KBAR(K)*DEL(K))/(4.*DEL(K))
      CME(1,1)=(B1*B1+C1*C1)*CONST
      CME(1,2)=(B1*B2+C1*C2)*CONST
      CME(1,3)=(B1*B3+C1*C3)*CONST
      CME(2,1)=CME(1,2)
      CME(2,2)=(B2*B2+C2*C2)*CONST
      CME(2,3)=(B2*B3+C2*C3)*CONST
      CME(3,1)=CME(1,3)
      CME(3,2)=CME(2,3)
      CME(3,3)=(B3*B3+C3*C3)*CONST

C
C
C
      FORM INFLUENCE MATRIX FOR STORAGE (MASS EQUATION)

      CONST=PI*DEL(K)/30.
      STME(1,1)=(4.*XCE(1)+6.*KBAR(K))*CONST
      STME(1,2)=(XCE(1)+XCE(2)+3.*KBAR(K))*CONST
      STME(1,3)=(XCE(1)+XCE(3)+3.*KBAR(K))*CONST
      STME(2,1)=STME(1,2)
      STME(2,2)=(4.*XCE(2)+6.*KBAR(K))*CONST
      STME(2,3)=(XCE(2)+XCE(3)+3.*KBAR(K))*CONST

```

```

      STME(3,1)=STME(1,3)
      STME(3,2)=STME(2,3)
      STME(3,3)=(4.*XCE(3)+6.*KBAR(K))*CONST
C
C ASSEMBLE SYSTEM EQUATIONS FOR MASS - THIS PROCESS TAKES THE
C VALUES FROM THE ELEMENT MATRICES (3X3) AND PUTS THEM IN THE
C PROPER LOCATION IN THE MASTER MATRIX (NMXNM).
C
      DO 130 IE=1,3
      I=NODE(K,IE)
      DO 130 JE=1,3
      J=NODE(K,JE)
      CMM(I,J)=CMM(I,J)+CME(IE,JE)
      STMM(I,J)=STMM(I,J)+STME(IE,JE)
130    CONTINUE
C
C RECYCLE FOR NEXT ELEMENT
C
140  CONTINUE
C
C SORT CONSTANT MATRICES FOR KNOWN VALUES AND FORM NEW MATRICES
C WHICH CAN BE SOLVED FOR UNKNOWN NODAL CONCENTRATIONS
C
      DO 133 I=1,NWSQC
      INQ=NQSC(I)
      CINIT(I)=CNC(INQ)
      DO 133 J=1,NNSC
      JNT=CNS(J)
      RHSL(I)=RHSL(I)-CMM(INQ,JNT)*CNC(JNT)
133    CONTINUE
      DO 134 I=1,NWSQC
      INQ=NQSC(I)
      DO 134 J=1,NWSQC
      JNQ=NQSC(J)
      STML(I,J)=STMM(INQ,JNQ)
      CML(I,J)=CMM(INQ,JNQ)
134    CONTINUE
C
C PERFORM MATRIX MANIPULATIONS TO UNCOUPLE EQUATIONS
C
      IDGT=5
      IJOB=2
      L=1
      CALL LINV2F(STML,NWSQC,NMAX,STMINV,IDGT,WKAREA,IER)
      CALL VMULFF(STMINV,CML,NWSQC,NWSQC,NWSQC,NMAX,NMAX,CMA,NMAX,IER)
      CALL EIGRF(CMA,NWSQC,NMAX,IJOB,CEVAL,CEVECC,NMAX,WKAREA,IER)
      DO 135 I=1,NWSQC
      DO 135 J=1,NWSQC
      CEVEC(I,J)=DREAL(CEVECC(I,J))
135    CONTINUE
      CALL LINV2F(CEVEC,NWSQC,NMAX,CEINV,IDGT,WKAREA,IER)
      CALL VMULFM(CEVEC,STML,NWSQC,NWSQC,NWSQC,NMAX,NMAX,CETC,NMAX,IER)
      CALL VMULFM(CEVEC,CML,NWSQC,NWSQC,NWSQC,NMAX,NMAX,CETC,NMAX,IER)
      CALL VMULFF(CETC,CEVEC,NWSQC,NWSQC,NWSQC,NMAX,NMAX,CETKE,NMAX,IER)

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      CALL VMULFF(CEINV,CINIT,NWSQC,NWSQC,L,NMAX,NMAX,CN,NMAX,IER)
      CALL VMULFM(CEVEC,RHSL,NWSQC,NWSQC,L,NMAX,NMAX,F,NMAX,IER)
C
C   CALL SUBROUTINE TO FORM CONC-DEPENDENT INFLUENCE MATRICES FOR ENERG
C
136   CALL CNCDEP(NE,NN,CP,CA,NODE,XC,D,TK,TM,STTM,CNC,
      *RHOA,YC,B,DEL,RBAR,CH)
C
C   SORT OUT KNOWN VALUES AND FORM NEW MATRICES WHICH CAN BE USED TO
C   SOLVE FOR UNKNOWN NODAL TEMPERATURES.
C
      DO 143 I=1,NN
      RHST(I)=0.
143   CONTINUE
141   DO 144 I=1,NWSQT
      INQ=NOST(I)
      TINIT(I)=T(INQ)
      DO 144 J=1,NNST
      JNT=NTS(J)
      RHST(I)=RHST(I)-TM(INQ,JNT)*T(JNT)
144   CONTINUE
      DO 145 I=1,NWSQT
      INQ=NOST(I)
      DO 145 J=1,NWSQT
      JNQ=NOST(J)
      STTL(I,J)=STTM(INQ,JNQ)
      TML(I,J)=TM(INQ,JNQ)
145   CONTINUE
C
C   INVERT CAPACITANCE MATRIX AND MULTIPLY BY STIFFNESS MATRIX GEN-
C   ERATION MATRIX: GET EIGENVALUES AND EIGENECTORS AND PERFORM MATRIX
C   MANIPULATIONS TO UNCOUPLE EQUATIONS
C
      IDGT=5
      IJOB=2
      L=1
      CALL LINV2F(STTL,NWSQT,NMAX,STLINV,IDGT,WKAREA,IER)
      CALL VMULFF(STLINV,TML,NWSQT,NWSQT,NWSQT,NMAX,NMAX,TMA,NMAX,IER)
      CALL EIGRF(TMA,NWSQT,NMAX,IJOB,TEVAL,TEVECC,NMAX,WKAREA,IER)
      DO 142 I=1,NWSQT
      DO 142 J=1,NWSQT
      TEVEC(I,J)=DREAL(TEVECC(I,J))
142   CONTINUE
      CALL LINV2F(TEVEC,NWSQT,NMAX,TEINV,IDGT,WKAREA,IER)
      CALL VMULFM(TEVEC,STTL,NWSQT,NWSQT,NWSQT,NMAX,NMAX,TETC,NMAX,IER)
      CALL VMULFF(TETC,TEVEC,NWSQT,NWSQT,NWSQT,NMAX,NMAX,TETCE,NMAX,IER)
      CALL VMULFM(TEVEC,TML,NWSQT,NWSQT,NWSQT,NMAX,NMAX,TETC,NMAX,IER)
      CALL VMULFF(TETC,TEVEC,NWSQT,NWSQT,NWSQT,NMAX,NMAX,TETKE,NMAX,IER)
      CALL VMULFF(TEINV,TINIT,NWSQT,NWSQT,L,NMAX,NMAX,TN,NMAX,IER)
      CALL VMULFM(TEVEC,RHST,NWSQT,NWSQT,L,NMAX,NMAX,G,NMAX,IER)
C
C   INITIALIZE FOR INTEGRATION SUBROUTINE FOR NODAL TEMPERATURES
C
      TT=TSTRT
      TST&T2=TSTRT

```

```

      TOL=0.001
      IND=1
C
C  CALL INTEGRATION SUBROUTINE FOR NODAL TEMPERATURES
C
      CALL DVERK(NWSQT,FCN2,TT,TN,TTEND,TOL,IND,C,NMAX,W,IER)
      IF(IND.LT.0.OR.IER.GT.0) GO TO 180
      DO 152 I=1,NWSQT
        T(NQST(I))=0.
      DO 152 J=1,NWSQT
        T(NQST(I))=T(NQST(I))+TEVEC(I,J)*TN(J)
152    CONTINUE
C
C  INITIALIZE FOR INTEGRATION SUBROUTINE FOR NODAL CONCENTRATIONS
C
      TT=TSTRT
      TSTRT2=TSTRT
      TOL=0.001
      IND=1
C
C  CALL INTEGRATION SUBROUTINE FOR NODAL CONCENTRATIONS
C
      CALL DVERK(NWSQC,FCN1,TT,CN,TTEND,TOL,IND,C,NMAX,W,IER)
      IF(IND.LT.0.OR.IER.GT.0) GO TO 180
      DO 176 I=1,NWSQC
        CNC(NQSC(I))=0.
      DO 176 J=1,NWSQC
        CNC(NQSC(I))=CNC(NQSC(I))+CEVEC(I,J)*CN(J)
176    CONTINUE
C
C  CHECK TO SEE IF CURRENT STEP IS ONE FOR WHICH COUTPUT IS DESIRED. IF
C  IT IS WRITE TIME, NODAL CONCENTRATIONS, AND NODAL TEMPERATURES TO
C  THE DATA FILE ON DISK.
C
      DO 174 I=1,NPRT
        IF(DABS(TTEND-PSTEP(I)).LE..0001) GO TO 175
174      CONTINUE
      GO TO 178
175      DO 177 J=1,NN
        WRITE(22,3500) TTEND,J,CNC(J),T(J)
177      CONTINUE
C
C  RESET INITIAL VALUE TO OLD INTEGRATION STEP
C  CHECK TO SEE WHICH INCREMENTAL TIME STEP TO USE AND INCREMENT
C  THE INTEGRATION STEP. CHECK TO SEE IF END TIME IS REACHED AND
C  EITHER STOP OR RETURN TO CONCENTRATION-DEPENDENT SUBROUTINE.
C
178      TSTRT=TTEND
      IF(TTEND.GE.CUTOFF) TSTEP=TSTEP2
      TTEND=TTEND+TSTEP
      IF(TTEND.GT.ENTM) GO TO 180
      GO TO 136
C
C *****
C

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C      FORMAT STATEMENTS
C
1035  FORMAT(5X,'NO. OF NODES=',I3,/,5X,'NO. OF ELEMENTS=',I3,/)
1036  FORMAT(5X,'INITIAL CONC',5X,'INITIAL TEMP',/)
1037  FORMAT(3X,F10.4,3X,F10.4)
1040  FORMAT(5X,'SUMMARY OF NODAL COORDINATES',/,
*7X,'I',12X,'X(I)',12X,'Y(I)',/)
1045  FORMAT(5X,I3,2(7X,F10.3))
1050  FORMAT(5X,'LISTING OF SYSTEM TOPOLOGY',/,5X,
*'ELEMENT NUMBER',20X,'NODE NUMBERS',/)
1055  FORMAT(5X,I3,10X,3(5X,I3))
1060  FORMAT(7X,'NODES WHERE CONCENTRATION IS SPECIFIED',
*//,5X,'I',5X,'NODE',5X,'CONCENTRATION',/)
1065  FORMAT(1X,I3,4X,I3,3X,F10.2)
1061  FORMAT(7X,'NODES WHERE TEMPERATURE IS SPECIFIED',
*//,5X,'I',5X,'NODE',5X,'TEMPERATURE',/)
1062  FORMAT(1X,I3,4X,I3,3X,F10.2)
1071  FORMAT(5X,'SPECIFIED DIFFUSION COEFFICIENT'
*//,2X,'ELEMENT NO.',5X,'DIFFUSION COEFFICIENT')
1070  FORMAT(5X,'SPECIFIED THERMAL CONDUCTIVITY'
*//,2X,'ELEMENT NO.',5X,'THERMAL CONDUCTIVITY')
1072  FORMAT(10X,'DENSITY',10X,'SPECIFIC HEAT',/,5X,'H2O VAPOR',
*5X,'AIR',3X,'H2O VAPOR',/)
1073  FORMAT(3X,F7.5,3X,F7.5,5X,F7.5)
1074  FORMAT(2X,F10.4,3X,F10.4,3X,F10.4,3X,F10.4)
1077  FORMAT(5X,'TIME STEP INFORMATION',/,2X,'END TIME',3X,'CUTOFF',
*3X,'SMALL TIME STEP',3X,'LARGE TIME STEP',/)
1075  FORMAT(5X,'PRINT STEP INFORMATION',/,2X,'NO.',5X,'TIME',/)
1076  FORMAT(5X,I3,2X,F10.4)
1080  FORMAT(5X,'
      NODES WHERE MASS FLUX IS SPECIFIED',
*      //,5X,'I',5X,'NODE',10X,'FLUX',/)
1081  FORMAT(5X,'
      NODES WHERE ENERGY FLUX IS SPECIFIED',
*      //,5X,'I',5X,'NODE',10X,'FLUX',/)
1085  FORMAT(5X,I3,3X,I3,10X,F12.3)
2016  FORMAT(1H1,5X,'GENERATION IS CONSTANT',/)
2017  FORMAT(1H1,5X,'GENERATION IS TIME-DEPENDENT',/)
3450  FORMAT(5X,'TIME',10X,'NODE',10X,'CNC',10X,'TEMP',/)
3500  FORMAT(1X,F10.2,5X,I3,5X,F10.6,5X,F10.6)
180   STOP
      END
C
C*****
C
C  SUBROUTINES*****
C
      SUBROUTINE FCN1(N,TT,CN,CPRIME)
      INTEGER N
      DOUBLE PRECISION CETG(63),CETCE(63,63),CETKE(63,63),F(63)
      DOUBLE PRECISION CPRIME(N),CN(N),TT,TSTRT
      COMMON /CNC/ CETCE,CETKE,CETG,F,TSTRT
C
C  CALL GENERATION SUBROUTINE MGEN WHICH IS SET UP BY THE USER TO
C  DETERMINE THE MASS GENERATION (RATE PER UNIT VOLUME FOR EACH
C  ELEMENT) FOR THE SPECIFIC APPLICATION.
C

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      IF(TT.EQ.TSTRT) CALL MGEN(TT,CETG)
      DO 10 I=1,N
      CPRIME(I)=(-CETKE(I,I)*CN(I)+CETG(I)+F(I))/CETCE(I,I)
10    CONTINUE
      RETURN
      END

C
C*****
C
      SUBROUTINE FCN2(N,TT,TN,TPRIME)
      INTEGER N
      DOUBLE PRECISION TETG(63),TETCE(63,63),TETKE(63,63),G(63)
      DOUBLE PRECISION TPRIME(N),TN(N),TT,TSTRT2
      COMMON /TEMP/ TETCE,TETKE,TETG,G,TSTRT2

C
C CALL GENERATION SUBROUTINE QGEN WHICH IS SET UP BY THE USER TO
C DETERMINE THE ENERGY GENERATION (RATE PER UNIT VOLUME FOR EACH
C ELEMENT) FOR THE SPECIFIC APPLICATION.
C
      IF(TT.EQ.TSTRT2) CALL QGEN(TT,TETG)
      DO 10 I=1,N
      TPRIME(I)=(-TETKE(I,I)*TN(I)+TETG(I)+G(I))/TETCE(I,I)
10    CONTINUE
      RETURN
      END

C
C SUBROUTINE CNCDEP*****
C
      SUBROUTINE CNCDEP(NE,NN,CP,CA,NCDE,XC,D,TK,TM,STTM,CNC,
      *RHOA,YC,B,DEL,RBAR,CH)
      DOUBLE PRECISION STTM(NN,NN),TM(NN,NN),CP,CA,RHOA,B1,B2,B3
      DOUBLE PRECISION C1,C2,C3
      DOUBLE PRECISION TME1(3,3),TME2(3,3),TME3(3,3),TME(3,3)
      DOUBLE PRECISION STTE2(3,3),STTE(3,3),STTE1(3,3),PI,CONST
      DOUBLE PRECISION DEL(NE),RBAR(NE),D(NE),TK(NE),B(NE,3),CNC(NN)
      DOUBLE PRECISION XCE(3),YCE(3),CH(NE,3),YC(NN),XC(NN),CNC(3)
      INTEGER NODE(NE,3)
      PI=3.1415927

C
C INITIALIZE THERMAL STIFFNESS AND THERMAL CAPACITANCE MATRICES
C
      DO 5 I=1,NN
      DO 5 J=1,NN
      TM(I,J)=0.
      STTM(I,J)=0.
5    CONTINUE

C
C START LOOP FOR ELEMENTS AND FORM ELEMENT NODAL EQUATIONS
C
      DO 10 K=1,NE
      XCE(1)=XC(NODE(K,1))
      XCE(2)=XC(NODE(K,2))
      XCE(3)=XC(NODE(K,3))
      YCE(1)=YC(NODE(K,1))

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```

YCE(2)=YC(NODE(K,2))
YCE(3)=YC(NODE(K,3))
B1=B(K,1)
B2=B(K,2)
B3=B(K,3)
C1=CH(K,1)
C2=CH(K,2)
C3=CH(K,3)

C
C FORM CONSTANT PORTION INFLUENCE MATRIX FOR TEMPERATURE
C
CONST=PI*TK(K)*RBAR(K)/(2.*DEL(K))
TME1(1,1)=(B1*B1+C1*C1)*CONST
TME1(1,2)=(B1*B2+C1*C2)*CONST
TME1(1,3)=(B1*B3+C1*C3)*CONST
TME1(2,1)=TME1(1,2)
TME1(2,2)=(B2*B2+C2*C2)*CONST
TME1(2,3)=(B2*B3+C2*C3)*CONST
TME1(3,1)=TME1(1,3)
TME1(3,2)=TME1(2,3)
TME1(3,3)=(B3*B3+C3*C3)*CONST

C
C FORM PARTIAL INFLUENCE MATRIX FOR STORAGE (ENERGY EQUATION)
C
CONST=PI*RHOA*CA*DEL(K)/30.
STTE1(1,1)=(4.*XCE(1)+6.*RBAR(K))*CONST
STTE1(1,2)=(XCE(1)+XCE(2)+3.*RBAR(K))*CONST
STTE1(1,3)=(XCE(1)+XCE(3)+3.*RBAR(K))*CONST
STTE1(2,1)=STTE1(1,2)
STTE1(2,2)=(4.*XCE(2)+6.*RBAR(K))*CONST
STTE1(2,3)=(XCE(2)+XCE(3)+3.*RBAR(K))*CONST
STTE1(3,1)=STTE1(1,3)
STTE1(3,2)=STTE1(2,3)
STTE1(3,3)=(4.*XCE(3)+6.*RBAR(K))*CONST

C
C GET NODAL CONCENTRATIONS FOR CURRENT ELEMENT
C
15 DO 20 IE=1,3
    I=NODE(K,IE)
    CNCE(IE)=CNC(I)
20 CONTINUE

C
C FORM CONCENTRATION DEPENDENT INFLUENCE MATRIX FOR TEMPERATURE
C
CONST=(PI*D(K)*CP)/(24.*DEL(K))*(B1*CNCE(1)+B2*CNCE(2)+B3*CNCE(3))
TME2(1,1)=(B1*(XCE(1)+3.*RBAR(K))*CONST
TME2(1,2)=(B2*(XCE(1)+3.*RBAR(K))*CONST
TME2(1,3)=(B3*(XCE(1)+3.*RBAR(K))*CONST
TME2(2,1)=(B1*(XCE(2)+3.*RBAR(K))*CONST
TME2(2,2)=(B2*(XCE(2)+3.*RBAR(K))*CONST
TME2(2,3)=(B3*(XCE(2)+3.*RBAR(K))*CONST
TME2(3,1)=(B1*(XCE(3)+3.*RBAR(K))*CONST
TME2(3,2)=(B2*(XCE(3)+3.*RBAR(K))*CONST
TME2(3,3)=(B3*(XCE(3)+3.*RBAR(K))*CONST
CONST=(PI*D(K)*CP)/(24.*DEL(K))*(C1*CNCE(1)+C2*CNCE(2)+C3*CNCE(3))

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TME3(1,1)=(C1*(XCE(1)+3.*RBAR(K)))*CCNST
TME3(1,2)=(C2*(XCE(1)+3.*RBAR(K)))*CCNST
TME3(1,3)=(C3*(XCE(1)+3.*RBAR(K)))*CCNST
TME3(2,1)=(C1*(XCE(2)+3.*RBAR(K)))*CCNST
TME3(2,2)=(C2*(XCE(2)+3.*RBAR(K)))*CCNST
TME3(2,3)=(C3*(XCE(2)+3.*RBAR(K)))*CCNST
TME3(3,1)=(C1*(XCE(3)+3.*RBAR(K)))*CCNST
TME3(3,2)=(C2*(XCE(3)+3.*RBAR(K)))*CCNST
TME3(3,3)=(C3*(XCE(3)+3.*RBAR(K)))*CCNST
C
C FORM CONCENTRATION DEPENDENT INFLUENCE MATRIX FOR STORAGE (ENERGY)
C
CONST=PI*CP*DEL(K)/90.
STTE2(1,1)=(CNCE(1)*(9.*XCE(1)+9.*RBAK(K))+CNCE(2)*(2.*XCE(1)
+XCE(2)+3.*RBAR(K))+CNCE(3)*(2.*XCE(1)+XCE(3)+3.*RBAR(K)))*CONST
STTE2(1,2)=(CNCE(1)*(2.*XCE(1)+XCE(2)+3.*RBAR(K))+CNCE(2)
*(XCE(1)+2.*XCE(2)+3.*RBAR(K))+CNCE(3)*(3.*RBAR(K)))*CONST
STTE2(1,3)=(CNCE(1)*(2.*XCE(1)+XCE(3)+3.*RBAR(K))+CNCE(2)*
*(3.*RBAR(K))+CNCE(3)*(XCE(1)+2.*XCE(3)+3.*RBAR(K)))*CONST
STTE2(2,1)=STTE2(1,2)
STTE2(2,2)=(CNCE(1)*(XCE(1)+2.*XCE(2)+3.*RBAR(K))+CNCE(2)*
*(9.*XCE(2)+9.*RBAR(K))+CNCE(3)*(2.*XCE(2)+XCE(3)+3.*RBAR(K)))*
*CONST
STTE2(2,3)=(CNCE(1)*(3.*RBAR(K))+CNCE(2)*(2.*XCE(2)+XCE(3)+3.*
RBAR(K))+CNCE(3)*(XCE(2)+2.*XCE(3)+3.*RBAR(K)))*CONST
STTE2(3,1)=STTE2(1,3)
STTE2(3,2)=STTE2(2,3)
STTE2(3,3)=(CNCE(1)*(XCE(1)+2.*XCE(3)+3.*RBAR(K))+CNCE(2)*(XCE
*(2)+2.*XCE(3)+3.*RBAR(K))+CNCE(3)*(9.*XCE(3)+9.*RBAR(K)))*CONST
C
C ASSEMBLE SYSTEM EQUATIONS FOR ENERGY
C
SITE(1,1)=STTE1(1,1)+STTE2(1,1)
SITE(1,2)=STTE1(1,2)+STTE2(1,2)
SITE(1,3)=STTE1(1,3)+STTE2(1,3)
SITE(2,1)=STTE1(2,1)+STTE2(2,1)
SITE(2,2)=STTE1(2,2)+STTE2(2,2)
SITE(2,3)=STTE1(2,3)+STTE2(2,3)
SITE(3,1)=STTE1(3,1)+STTE2(3,1)
SITE(3,2)=STTE1(3,2)+STTE2(3,2)
SITE(3,3)=STTE1(3,3)+STTE2(3,3)
TME(1,1)=TME1(1,1)+TME2(1,1)+TME3(1,1)
TME(1,2)=TME1(1,2)+TME2(1,2)+TME3(1,2)
TME(1,3)=TME1(1,3)+TME2(1,3)+TME3(1,3)
TME(2,1)=TME1(2,1)+TME2(2,1)+TME3(2,1)
TME(2,2)=TME1(2,2)+TME2(2,2)+TME3(2,2)
TME(2,3)=TME1(2,3)+TME2(2,3)+TME3(2,3)
TME(3,1)=TME1(3,1)+TME2(3,1)+TME3(3,1)
TME(3,2)=TME1(3,2)+TME2(3,2)+TME3(3,2)
TME(3,3)=TME1(3,3)+TME2(3,3)+TME3(3,3)
DO 25 IE=1,3
I=NODE(K,IE)
DO 25 JE=1,3
J=NODE(K,JE)
TM(I,J)=TM(I,J)+TME(IE,JE)

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```

      STTM(I,J)=STTM(I,J)+STTE(IE,JE)
25      CONTINUE
10      CONTINUE
      CFLAG=1
      RETURN
      END

C
C*****
C
C THE FOLLOWING SUBROUTINES ARE TO BE SET UP BY THE USER FOR EACH
C SPECIFIC APPLICATION. IT IS IMPORTANT TO REALIZE THAT SINCE THE
C MODEL DOES NOT ACCOUNT FOR CHANGES IN PHASE, THE USER IS RESPONSIBLE
C FOR SPECIFYING THE APPROPRIATE ENERGY AND MASS GENERATION WHICH
C SATISFY THE ENERGY AND MASS BALANCE FOR THE SYSTEM.
C
C SUBROUTINE MGEN*****
C
C SUBROUTINE FOR MASS GENERATION WHICH IS CALLED DURING EACH
C INTEGRATION STEP FROM SUBROUTINE FCN1. THE USER MUST SUPPLY
C THE CODING FOR THE RATE OF GENERATION PER UNIT VOLUME IN EACH
C ELEMENT FOR A SPECIFIC APPLICATION. THESE VALUES SHOULD BE
C STORED IN THE ARRAY MG(K) WHICH IS DIMENSIONED TO THE NUMBER
C OF ELEMENTS IN THE GRID. ONCE THIS ARRAY IS FORMED, THE PRO-
C GRAM ACCOUNTS FOR THE DIFFUSION OF THIS MASS INTO THE AIR.
C
C
C SUBROUTINE MGEN(TT,CETG)
      DOUBLE PRECISION DEL(80),XC(63),XCE(3),RBAR(80),CEVEC(63,63)
      DOUBLE PRECISION PI,CONST,TEVEC(63,63),CETG(63),TT
      REAL*8 MGM(63),MGME(3),MG(80),MGML(63)
      INTEGER NODE(80,3),NUSC(63),NQST(63),IER,NN,NE,NWSCT,NWSSC
      COMMON /GEN/ CEVEC,TEVEC,RBAR,DEL,XC,NUSC,NQST,NWSSC,NWSCT,NN,NE
      *,NODE,IER
      PI=3.1415927
      L=1
      NMAX=NN
      DO 5 I=1,NN
      MGM(I)=0.
5      CONTINUE
C
C START LOOP FOR ELEMENTS AND FORM ELEMENT NODAL EQUATIONS
C
      DO 10 K=1,NE
      XCE(1)=XC(NODE(K,1))
      XCE(2)=XC(NODE(K,2))
      XCE(3)=XC(NODE(K,3))
C
C USER SUPPLIED CODING FOR ELEMENT MASS GENERATION (RATE PER UNIT
C VOLUME.
C
C*****
C
      MG(K)=0.
C
C*****

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```

C
C   FORM INFLUENCE MATRIX FOR MASS GENERATION
C
      CONST=PI*MG(K)*DEL(K)/2.
      MGME(1)=CONST*(RBAR(K)+XCE(1)/3.)
      MGME(2)=CONST*(RBAR(K)+XCE(2)/3.)
      MGME(3)=CONST*(RBAR(K)+XCE(3)/3.)
C
C   ASSEMBLE SYSTEM EQUATIONS
C
      DO 15 IE=1,3
      I=NODE(K,IE)
      MGM(I)=MGM(I)+MGME(IE)
15    CONTINUE
10    CONTINUE
      DO 20 I=1,NWSQC
      INQ=NQSC(I)
      MGML(I)=MGM(INQ)
20    CONTINUE
      CALL VMULFM(CEVEC,MGML,NWSQC,NWSQC,L,NMAX,NMAX,CETG,NMAX,IER)
      RETURN
      END
C
C   SUBROUTINE QGEN*****
C
C   SUBROUTINE FOR HEAT GENERATION WHICH IS CALLED DURING EACH
C   INTEGRATION STEP FROM SUBROUTINE FCN2. THE USER MUST SUPPLY
C   THE CODING FOR THE RATE OF GENERATION PER UNIT VOLUME IN EACH
C   ELEMENT FOR A SPECIFIC APPLICATION. THESE VALUES SHOULD BE
C   STORED IN THE ARRAY QG(K) WHICH IS DIMENSIONED TO THE NUMBER
C   OF ELEMENTS IN THE GRID. ONCE THIS ARRAY IS FORMED, THE PRO-
C   GRAM ACCOUNTS FOR THE DIFFUSION OF THIS HEAT INTO THE AIR.
C
      SUBROUTINE QGEN(TT,TETG)
      DOUBLE PRECISION DEL(80),XC(63),XCE(3),RBAR(80),CEVEC(63,63)
      DOUBLE PRECISION PI,CONST,TEVEC(63,63),TETG(63),TT
      DOUBLE PRECISION QGM(63),QGME(3),QG(80),QGML(63)
      INTEGER NODE(80,3),NQSC(63),NQST(63),IER,NN,NE,NWSCT,NWSC
      COMMON /GEN/ CEVEC,TEVEC,RBAR,DEL,XC,NQSC,NQST,NWSCT,NN,NE
      *.NODE,IER
      PI=3.1415927
      L=1
      NMAX=NN
      DO 5 I=1,NN
      QGM(I)=0.
5     CONTINUE
C
C   START LOOP FOR ELEMENTS AND FORM ELEMENT NODAL EQUATIONS
C
      DO 10 K=1,NE
      XCE(1)=XC(NODE(K,1))
      XCE(2)=XC(NODE(K,2))
      XCE(3)=XC(NODE(K,3))
C
C   USER SUPPLIED CODING FOR ELEMENT MASS GENERATION (RATE PER UNIT

```

```

C  VOLUME.
C
C *****
C
      QG(K)=0.
C
C *****
C
C  FORM INFLUENCE MATRIX FOR MASS GENERATION
C
      CONST=P1*QG(K)*DEL(K)/2.
      QGME(1)=CONST*(RBAR(K)+XCE(1)/3.)
      QGME(2)=CONST*(RBAR(K)+XCE(2)/3.)
      QGME(3)=CONST*(RBAR(K)+XCE(3)/3.)
C
C  ASSEMBLE SYSTEM EQUATIONS
C
      DO 15 IE=1,3
      I=NODE(K,IE)
      QGM(I)=QGM(I)+QGME(IE)
15  CONTINUE
10  CONTINUE
      DO 20 I=1,NWSQT
      INQ=INQST(I)
      QGML(I)=QGM(INQ)
20  CONTINUE
      CALL VMULFM(TEVEC,QGML,NWSQT,NWSQT,L,NMAX,NMAX,TETG,NMAX,IER)
      RETURN
      END

```


SUMMARY OF VARIABLES AND ARRAYS

<u>Description</u>	<u>Mass</u>	<u>Energy</u>
1. Dependent variable after integration	CNC	T
2. Derivative of dependent variable with time	CPRIME	TPRIME
3. Sorted array of dependent variables which are solved for during integration	CN	TN
4. Sorted initial values of dependent variables used to get initial values of TN and CN	CINIT	TINIT
5. Element stiffness matrix constant portion concentration-dependent portion	CME	TME TME1 TME2,TME3
6. Assembled stiffness matrix	CMM	TM
7. Sorted assembled stiffness matrix	CML	TML
8. Element capacitance matrix constant portion concentration-dependent portion	STME	STTE STTE1 STTE2
9. Assembled capacitance matrix	STMM	STMM
10. Sorted assembled capacitance matrix	STML	STTL
11. Generation (rate/volume)	MG	QG
12. Element influence matrix for generation	MGME	QGME
13. Assembled influence matrix for generation	MGM	QGM
14. Sorted assembled influence matrix for gen.	MGML	QGML
15. Element nodal temperature		TE
17. Diffusion coefficient	D	
18. Thermal conductivity		TK

<u>Description</u>	<u>Mass</u>	<u>Energy</u>
19. Sorted right-hand-side matrix (fluxes)	RHSL	RHST
20. Inverse of sorted assembled capacitance matrix	STMINV	STLINV
21. Stiffness matrix times inverse of capacitance matrix	CMA	TMA
22. Eigenvalues of (21)	CEVAL	TEVAL
23. Eigenvectors of (21)	CEVEC	TEVEC
24. Inverse of eigenvectors	CEINV	TEINV
25. Product of eigenvectors and capacitance matrix (also product of eigenvectors and stiffness matrix - intermediate calculations using common memory)	CETC	TETC
26. Product of (25) and eigenvectors	CETCE	TETCE
27. Product of (19) and eigenvectors	F	G
28. Product of sorted generation matrix and eigenvectors	CETG	TETG
29. Number of nodes with specified conc/temp	NNSC	NNST
30. List of nodes with specified conc/temp	CNS	NTS
31. Specified temp/conc	NNCNC	TNT
32. Node with specified temp/conc	NCNC	NT
33. Specified flux	KQC	KQT
34. Number of nodes with specified flux	NWSQC	NWSQT
35. List of nodes with specified flux	NQSC	NQST
36. Number of nodes in grid	NN	NN
37. Number of elements in grid	NE	NE
38. Specified flux	Q	Q

<u>Description</u>	<u>Mass</u>	<u>Energy</u>
39. Area of element	DEL	DEL
40. Volume of element	VOL	VOL
41. List of nodes for each element	NODE	NODE
42. Element nodal r-coordinate	XCE	XCE
43. Element nodal z-coordinate	YCE	YCE
44. Assembled list of nodal r-coordinates	XC	XC
45. Assembled list of nodal z-coordinates	YC	YC
46. R-coordinate of element centroid	RBAR	RBAR
47. Z-coordinate of element centroid	ZBAR	ZBAR
48. Ending time for problem	ENTM	ENTM
49. Right side of integration interval	TTEND	TTEND
50. Initial time (left side) of integration interval	TSTRT	TSTRT
51. Cutoff value for partitioning problem into two parts: for $0 < t < \text{CUTOFF}$ - use small steps for $\text{CUTOFF} < t < \text{ENTM}$ - use large time steps	CUTOFF	CUTOFF
52. Value of small time step	TSTEP	TSTEP
53. Value of large time step	TSTEP2	TSTEP2
54. Time steps used within integration sub-routine	TT	TT
55. Convergence criteria for integration	TOL	TOL
56. Constants for elements	A1,A2,A3, B1,B2,B3 C1,C2,C3	A1,A2,A3, B1,B2,B3 C1,C2,C3
57. Master matrix of constants	B,CH	B,CH

<u>Description</u>	<u>Mass</u>	<u>Energy</u>
58. Density of air	RHOA	RHOA
59. Specific heat of air	CA	CA
60. Specific heat of water vapor	CP	CP
61. Initial nodal temp/conc	CNCO,TO	CNCO,TO
62. Number of times for printout	NPRT	NPRT
63. Values of time for printout	PSTEP	PSTEP
64. Work area matrix for IMSL subroutines	WKAREA	WKAREA
65. Work space matrix for integration subroutine	W	W
66. Communications vector for integration subroutine	C	C
67. Error parameter for IMSL subroutines	IER	IER
68. Parameter for eigenvalue/eigenvector subroutine	IJOB	IJOB
69. Accuracy parameter for IMSL subroutines	IDGT	IDGT
70. Index parameter for integration subroutine	IND	IND

VITA

Joel G. Hall was born in Knoxville, Tennessee on March 26, 1961. He attended elementary schools in that city and graduated from Farragut High School in June 1979. He immediately entered The University of Tennessee and received a Bachelor of Science degree in Agricultural Engineering in December 1984. In the spring of 1985 he accepted a graduate research assistantship at The University of Tennessee, Knoxville and began study toward a Master's degree with a major in Agricultural Engineering. This degree was awarded in December 1985.

The author is a member of Tau Beta Pi, Phi Kappa Phi, and the American Society of Agricultural Engineers. He was awarded a Tau Beta Pi Fellowship for graduate study in engineering in 1984. After graduation Mr. Hall will be employed by CH2M HILL in Gainesville, Florida.