CHAPTER II

MATHEMATICAL FORMULATION OF TRANSIENT TEMPERATURE DISTRIBUTION IN BOTH CONTINUOUS AND DIFFERENCE FORM

In this chapter the transient temperature problem is formulated as the continuous solution to a partial differential equation. Also, a generalized version of the MacNeal-Longwell (9) approximate method is derived, and the equations suitable for stepping out the solution are shown. Further, the forms of an analytic solution of both the partial differential equation, and of the system of linear difference equations that result from the approximation, are shown. The dependence on the differencing parameters of the quantities in the solution to the difference approximation is indicated. Throughout this discussion the emphasis is on showing the likeness and analogies between the continuous and approximate methods. These analogies are in the derivation of the equations, in the properties of the operators occurring in the equations, in the form of the solutions for the equations, and in the properties of the terms in the equations.

(A) CONTINUOUS OR EXACT FORMULATION

The diffusion equation is simply derived, starting with Fourier's law for heat conduction in one direction

$$\dot{q} = - k \frac{\partial T}{\partial x} \tag{II-1}$$

or, in general, in three dimensions

$$\vec{\dot{q}} = - k \overrightarrow{\nabla T} \tag{II-2}$$

Applying the law of conservation of energy to a differential volume element which contains no sources or sinks, the net energy into the differential volume equals the accumulation, or, in vector notation, the time rate of change of temperature is proportional to the negative of the divergence of the heat flux.

$$\sigma C_p \frac{\partial T}{\partial \theta} = - \vec{\nabla} \cdot \vec{\dot{q}} \tag{II-3}$$

Combining equations II-2 and II-3 gives the diffusion equation,

$$\sigma C_p \frac{\partial T}{\partial \theta} = \vec{\nabla} \cdot k \vec{\nabla} T \tag{II-4}$$

which applies to the interior of the solid and is linear if k, σ, and C_p do not depend on T. For convenience, dimensionless variables are usually introduced which for three space dimensions are

$$\tau = \left(\frac{k}{\sigma C_p}\right)_0 \frac{\theta}{L^2} = K_0 \frac{\theta}{L^2} \tag{II-5}$$

$$\xi = x/L \tag{II-6}$$

$$\eta = y/L \tag{II-7}$$

$$\zeta = z/L \tag{II-8}$$

The diffusion equation in terms of these dimensionless variables becomes

$$\frac{\partial T}{\partial \tau} = \frac{1}{C_p \sigma K_0} \vec{\nabla}' \cdot k \vec{\nabla}' T \tag{II-9}$$

where $(1/L)\ \nabla' = \nabla$

For the one- and two-dimensional cases where the thermal conductivity and volumetric capacity are constant the equations are

$$\frac{\partial T}{\partial \tau} = \frac{\partial^2 T}{\partial \xi^2} \tag{II-10}$$

$$\frac{\partial T}{\partial \tau} = \frac{\partial^2 T}{\partial \xi^2} + \frac{\partial^2 T}{\partial \eta^2} \tag{II-11}$$

To uniquely define the solution temperature T, the initial temperature distribution and the boundary conditions must be specified. For the two-dimensional case the initial distribution would be of the form

$$T = T(\xi, \eta, 0) \qquad \tau = 0 \tag{II-12}$$

For many practical problems the boundary conditions are often of the type

$$h[T_f(\xi_B, \eta_B, \tau) - T(\xi_B, \eta_B, \tau)] = -k \frac{\partial T}{\partial n}(\xi_B, \eta_B, \tau) \qquad \text{(II-13)}$$

$$0 \leq h \leq \infty$$

where ξ_B and η_B are the coordinates of the boundary of the solid, and where n is normal to the boundary directed toward the interior. The heat-transfer coefficient is always positive and may vary from zero (adiabatic condition) to infinity (a specified boundary temperature). For the one-dimensional case the initial condition would be a function only of ξ, and the boundary condition would give equations like II-13 for two values of ξ.

The Laplacian operator* $\nabla \cdot k \nabla$ or $\nabla' \cdot k \nabla'$ itself and the combination of Laplacian operator together with its boundary conditions have several important mathematical properties. The Laplacian operator is a stable operator, or, equivalently, it tends to minimize the energy at a point. When the Laplacian operator and its boundary conditions are considered together, this property has the physical meaning that, for boundary conditions which represent a finite amount of energy, the temperature remains bounded. Mathematically this is expressed as a negative property meaning that, for homogeneous

* Although in this thesis the operators $\nabla \cdot k \nabla$ or $\nabla' \cdot k \nabla'$ are called Laplacian operators, the Laplacian operator is usually defined as ∇^2.

boundary conditions (equation II-13 with T_f of zero), the following volume integral is negative (5).

$$\iiint_V T\nabla \cdot k\nabla T \, dV < 0 \tag{II-14}$$

where T is any smooth function that satisfies a homogeneous boundary condition (equation II-13 with $T_f(\xi_B, \eta_B) = 0$) .

$$k \frac{\partial T}{\partial n}(\xi_B, \eta_B) - hT(\xi_B, \eta_B) = 0 \tag{II-15}$$

This means essentially that the characteristic roots of the operator are negative; and the transient part of the solution is a sum of negative exponentials. This result can be generalized, using theorems found in Carslaw and Jaeger (1), by superposition to nonhomogeneous boundary conditions where T_f is a non-zero function of the boundary coordinates, but constant with time, and by Duhamel's Theorem (1) to cases where T_f is a function both of boundary coordinates and time. The fluid temperature function can be considered to be analogous to a forcing function for a stable linear ordinary differential equation. The second important property is that the Laplacian operator is symmetric or self-adjoint. Physically this means that the thermal conductance in one direction is the same as in the reverse direction. For the operator and the nonhomogeneous boundary condition, equation II-13, this property is stated mathematically in terms of a volume integral.

$$\iiint_V T^{*} \nabla \cdot k \nabla T^{**} dV = \iiint_V T^{**} \nabla \cdot k \nabla T^{*} dV \qquad \text{(II-16)}$$

where T^{*} and T^{**} are functions that fit the homogeneous boundary condition, equation II-15. These are properties that the approximate formulation retains.

(B) CONTINUOUS SOLUTION

The solution for the linear one-dimensional problem (equation II-10) with linear boundary conditions (equation II-13) is written symbolically as:

$$T(\xi,\tau) = T_P(\xi,\tau) - \sum_{j=1}^{\infty} a_j b_j(\xi) e^{-\upsilon_j^2 \tau} \qquad \text{(II-17)}$$

$$0 \le \xi \le 1$$

$$\tau \ge 0$$

(Here and in the following discussion ξ need not be a Cartesian coordinate.) In this equation $T_P(\xi,\tau)$ is a true steady-state solution that is not a function of time if the fluid temperature is constant; or it is a quasi-steady-state solution if the fluid temperature changes with time and, in this case, is related to Duhamel's Theorem. The terms after the summation sign are the transient solution and this part of the solution is related to the problem of zero fluid temperature and an arbitrary initial temperature distribution. In the transient solution the υ_j's are an infinite number of real roots to the characteristic equation which depends upon the boundary equations. Since the υ_j's are real, $-\upsilon_j^2$ is negative, and the exponentials go to zero with increasing time. The $b_j(\xi)$ is the eigenfunction that corresponds to υ_j; these functions are orthogonal over the range of ξ with respect to a weighting function

$$\int_0^1 \sigma(\xi)\, b_j(\xi)\, b_\rho(\xi)\, d\xi = \delta_{j,\rho} \qquad \text{(II-18)}$$

$$j, \rho = 1, 2, \ldots \infty$$

The a_j's are the Fourier coefficients determined with the orthogonality relationship so that the expression fits the initial temperature distribution.

$$a_j = \int_0^1 \sigma(\xi)\, b_j(\xi)\, [T(\xi, 0) - T_P(\xi, 0)]\, d\xi \qquad \text{(II-19)}$$

Although the solution above is shown specifically for the heat-transfer coefficient boundary condition, equation II-13, the above form is also true for other problems, for which the solution may be found by the separation of variables technique, or for which the Laplace transform of the solution has only poles for singularities. Consequently the above form holds for many of the commonly encountered problems. The main problem it does not appear to apply to is where ξ extends to infinity (semi-infinite solid); however, by replacing the summation with an integration, together with other appropriate manipulations, a form very similar to equation II-17 is found which does apply.

For a two-dimensional problem of equation II-11 the above arguments can be used to show that the solution is in the form:

$$T(\xi, \eta, \tau) = T_P(\xi, \eta, \tau) - \sum_{j=1}^{\infty} \sum_{j=1}^{\infty} a_{ij}\, b_{ij}(\xi, \eta) e^{-\nu_{ij}^2 \tau} \qquad \text{(II-20)}$$

Either to compare the continuous solution with an approximate solution, or to calculate a continuous solution for a case where it is known, a vector-matrix form for the solution is sometimes preferred. Assuming that the temperature at S points within the solid is desired, an S-dimensional "continuous temperature vector" can be defined with its i^{th} element found by evaluating equation II-17 or II-20 at the coordinate of the i^{th} point. Also, because the infinite sum is over damped exponentials, to obtain a certain degree of accuracy for any time greater than zero. only a finite number of the largest exponential terms need be considered. If this number is J the continuous solution vector for a one-dimensional problem can be written as

$$T(\tau) = T_P(\tau) - B\, e^{-\upsilon^2 \tau}\, a \qquad \text{(II-21)}$$

where $T_P(\tau)$ is an S-dimensional vector of particular solutions; B is an S by J matrix whose j^{th} column is $b_j(\xi)$ evaluated for the appropriate ξ's; $e^{-\upsilon^2 \tau}$ is a diagonal matrix with the j^{th} diagonal element $e^{-\upsilon_j^2 \tau}$; and a is a J-dimensional vector of Fourier coefficients a_j. The continuous solution equation II-20 for the two-dimensional problem also can be put into exactly the same vector-matrix form as above, equation II-21.

(C) APPROXIMATE FORMULATION

The difference equations that are used to approximate the partial differential equation are usually derived by either of two methods: first, directly from physical considerations, and second, from a Taylor series expansion of the temperature function. The series method is also very useful in the analysis of errors introduced by replacing the differential equation by a difference approximation, and is used in Chapter V. Here the approximations are derived directly from an energy balance for a two-dimensional problem using an asymmetric distribution of points following MacNeal (8) and Longwell (9). Although this system derived for the irregular distribution of temperature points might not be entirely satisfactory, as discussed in Chapter V, it results in a useful general matrix-vector formulation that can be considered to be independent of some of the rules for finding the actual matrix elements, and which reduces to the usual approximations for a regular arrangement of nodes. Further, although only the two-dimensional case is derived, the concepts of one- and three-dimensional cases are similar; however, in practice, the three-dimensional case is sometimes difficult to visualize.

Following MacNeal's (8) rules for two-dimensional flow, points are selected within the cross-section. Lines are drawn from each point to surrounding points in such a manner that the lines do not intersect. It must be possible to connect the points with physically

realizable resistors, which means that the internal angles must not be obtuse in triangles. If necessary, the points should be rearranged to meet these restrictions. Next, perpendicular bisectors are constructed for each line between the points; if the above rules are followed these bisectors will meet at a point, and the network will appear as in Figure III-1. A temperature node is defined for convenience as a point mass having a heat capacity and thermal conductances to surrounding nodes based on the physical and geometrical properties of the surrounding area.

Considering the i^{th} node, the thermal conductance between this and an adjacent node j is given by:

$$\frac{\dot{q}_{ij}}{t_i - t_j} = \frac{k\, r_{ij}}{\ell_{ij}} \qquad i = 1, 2, \ldots, R \qquad \text{(II-22)}$$

The volume or area of unit thickness for the two-dimensional case for the i^{th} node is

$$\text{Area}_i = \tfrac{1}{4} \sum_{\substack{j=1 \\ j \neq i}}^{R} r_{ij}\, \ell_{ij} \qquad i = 1, 2, \ldots, R \qquad \text{(II-23)}$$

where r_{ij} is zero if there is no connection between i and j; r_{ii} and ℓ_{ii} have no meaning; and the summation is over all nodes surrounding the i^{th} node. Thus, setting the accumulation of energy at the node equal to the net flux in, we may write an ordinary differential equation for each node,

$$\frac{\sigma C_p}{4}\left(\sum_{\substack{j=1\\ j\neq i}}^{R} r_{ij}\,\ell_{ij}\right)\frac{dt_i}{d\theta} = k\sum_{\substack{j=1\\ j\neq i}}^{R}\frac{r_{ij}}{\ell_{ij}}(t_j - t_i) \qquad \text{(II-24)}$$

$$i = 1, 2, \ldots, R$$

Consequently, the partial differential equation has been replaced with a system of ordinary differential equations which are suitable for solution on an analog computer. Following Longwell's (9) derivation, a dimensionless heat capacity A_i and a dimensionless conductance are introduced.

$$A_i = \frac{\sigma C_p (\text{Area})_i}{(\sigma C_p)_0 L^2} = \frac{\sigma C_p}{4(\sigma C_p)_0}\sum_{j=1}^{R}\frac{r_{ij}\,\ell_{ij}}{L^2} \qquad \text{(II-25)}$$

$$i = 1\ 2\ .\ .\ ., R$$

$$y_{ij} = \frac{k}{k_0}\frac{r_{ij}}{\ell_{ij}} \qquad i,j = 1, 2, \ldots, R \qquad \text{(II-26)}$$

Substitution gives

$$\sum_{\substack{j=1\\ j\neq i}}^{R} y_{ij}(t_j - t_i) = A_i\frac{dT_i}{d\tau} \qquad i = 1, 2, \ldots, R \qquad \text{(II-27)}$$

Now departing from both MacNeal's (8) and Longwell's (9) derivations, the system of equations may be summarized in matrix form:

$$\left[\begin{array}{cccc|ccc} A_1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & A_2 & \cdots & 0 & 0 & \cdots & 0 \\ \cdot & \cdot & & \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & \cdot & & \cdot \\ 0 & 0 & \cdots & A_S & 0 & \cdots & 0 \\ \hline 0 & 0 & \cdots & 0 & A_{S+1} & \cdots & 0 \\ \cdot & \cdot & & \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & \cdot & & \cdot \\ 0 & 0 & \cdots & 0 & 0 & & A_R \end{array}\right] \frac{d}{d\tau} \left(\begin{array}{c} t_1 \\ t_2 \\ \cdot \\ \cdot \\ \cdot \\ t_S \\ \hline t_{S+1} \\ \cdot \\ \cdot \\ \cdot \\ t_R \end{array}\right) - \qquad \text{(II-28)}$$

$$\left[\begin{array}{cccc|ccc} -\sum_{\substack{j=2 \\ j\neq 1}}^{R} y_{1j} & y_{12} & \cdots & y_{1S} & y_{1S+1} & \cdots & y_{1R} \\ y_{12} & -\sum_{\substack{j=1 \\ j\neq 2}}^{R} y_{2j} & \cdots & y_{2S} & y_{2S+1} & \cdots & y_{2S} \\ \cdot & \cdot & & \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & \cdot & & \cdot \\ y_{1S} & y_{2S} & \cdots & -\sum_{\substack{j=1 \\ j\neq S}}^{R} y_{Sj} & y_{SS+1} & \cdots & y_{SR} \\ \hline y_{1S+1} & y_{2S+1} & \cdots & y_{SS+1} & -\sum_{\substack{j=1 \\ j\neq S+1}}^{R} y_{S+1j} & \cdots & y_{S+1R} \\ \cdot & \cdot & & \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot & \cdot & & \cdot \\ y_{1R} & y_{2R} & \cdots & y_{SR} & y_{S+1R} & \cdots & -\sum_{\substack{j=1 \\ j\neq R}}^{R} y_{Rj} \end{array}\right] \left(\begin{array}{c} t_1 \\ t_2 \\ \cdot \\ \cdot \\ \cdot \\ t_S \\ \hline t_{S+1} \\ \cdot \\ \cdot \\ \cdot \\ t_R \end{array}\right)$$

Since some of the nodes represent boundary nodes, their temperatures are known as a function of time. Assuming that the boundary nodes are (S+1) to R, we may rewrite the matrix without the equations for nodes (S+1) to R. Carrying this out, and simplifying the equations by partitioning the matrices and temperature vector, gives

$$\begin{bmatrix} A_1 & 0 & \cdots & 0 \\ 0 & A_2 & \cdots & 0 \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ 0 & 0 & \cdots & A_S \end{bmatrix} \frac{d}{d\tau} \begin{pmatrix} t_1 \\ t_2 \\ \cdot \\ \cdot \\ \cdot \\ t_S \end{pmatrix} = \begin{bmatrix} -\sum_{\substack{j=2 \\ j\neq 1}}^{R} y_{1j} & y_{12} & \cdots & y_{1S} \\ y_{12} & -\sum_{\substack{j=1 \\ j\neq 2}}^{R} y_{2j} & \cdots & y_{2S} \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ \cdot & \cdot & & \cdot \\ y_{1S} & y_{2S} & \cdots & -\sum_{\substack{j=1 \\ j\neq S}}^{R} y_{Sj} \end{bmatrix} \begin{pmatrix} t_1 \\ t_2 \\ \cdot \\ \cdot \\ \cdot \\ t_S \end{pmatrix} \tag{II-29}$$

$$+ \begin{bmatrix} y_{1\,S+1} & \cdots & y_{1R} \\ y_{2\,S+1} & \cdots & y_{2R} \\ \cdot & & \cdot \\ \cdot & & \cdot \\ \cdot & & \cdot \\ y_{R\,S+1} & \cdots & y_{RR} \end{bmatrix} \begin{pmatrix} t_{S+1} \\ \cdot \\ \cdot \\ \cdot \\ t_R \end{pmatrix}$$

which is written equivalently in vector-matrix form as

$$A \frac{d}{d\tau} t = Yt + Y_B t_B \tag{II-30}$$

where the two equations serve to define the several matrices and vectors. The A matrix, because each diagonal element is a positive

non-zero element, is a positive definite matrix. The Y matrix is a symmetric matrix that represents a network of thermal resistors; thus, it is a negative definite matrix.

Although the above equation was derived specifically for points located on the boundary, whose temperature is known as a function of time, generalizations to other types of linear boundary conditions can be made. This can be done, for example, in the case of the solid surrounded by a fluid with a heat-transfer coefficient h, or for a specified flux per unit area, merely by modifying the energy balances appropriately for the effect on nodes on or close to the boundary. If the boundary condition equations involve a heat-transfer coefficient, the Y and Y_R matrices contain the heat-transfer coefficient. This condition is thoroughly discussed later. If the flux is specified, then there is no boundary conductance, the Y matrix is the same as for zero h or an adiabatic condition, and $Y_B\ t_B$ is replaced directly with the known flux in to each node per unit time. Also, for the equation in the above form, it is easy to see that the boundary temperature vector (or flux vector) is the nonhomogeneous part of the equation and the boundary temperature vector t_B can be considered a forcing function or input disturbance.

Now solving equation II-30 for $\frac{d}{d\tau} t$ to put it in a form similar to the partial differential equation, there is obtained after defining two new matrices:

$$\frac{d}{d\tau} t = \frac{Y}{A} t + \frac{Y_B}{A} t_B \tag{II-31}$$

where $$\frac{Y}{A} = A^{-1} Y \text{ and } \frac{Y_B}{A} = A^{-1} Y_B \tag{II-32}$$

At this point the Laplacian operator $(1/K_0 C_p \sigma) \nabla' k \nabla'$ and its boundary conditions which apply to all points within and on the boundary of the solid have been replaced with matrix operators Y/A and Y/A_B, which apply at a finite number of points within and on the solid boundary. For the i^{th} point, we have

$$\frac{1}{K_0 \sigma C_p} \nabla' k \nabla' T_i \approx \frac{1}{A_i} \sum_{j=1}^{R} y_{ij}(t_j - t_i) \tag{II-33}$$

$$i = 1, \ldots, S$$

The matrix Y/A does retain both the stable or negative property and the symmetric property of the Laplacian operator. First the Y/A matrix as defined by the above rules can be shown to be a negative definite or negative semi-definite matrix and so has all negative eigenvalues, and a finite sum analogous to the volume integral is always negative. The transient solution to the system of ordinary differential equations is then a sum of damped exponentials giving a stable solution. As the Y/A matrix is not a symmetric matrix (except for the important case when all the A_i's are equal), it might appear that the symmetric property is lost; however, the following discussion shows that the matrix operator is symmetric in the same sense as the

Laplacian is symmetric. In the volume integral that defines this property, the value of $\nabla' . k \nabla' T$ is weighted by the differential volume for which it applies; consequently, an equivalent weighting is introduced when the Laplacian and the differential volume element, dV, are expressed in cylindrical or other orthogonal curvilinear coordinates. Thus, in the finite sum over the volume that is the discrete analog of the volume integral, the A_i's are used as the weighting for the i^{th} point. This sum is then

$$\sum_{i=1}^{S} A_i t_i^* \left[\frac{1}{A_i} \sum_{j=1}^{S} y_{ij} (t_j^{**} - t_i^{**}) \right] = \sum_{i=1}^{S} t_i^* \sum_{j=1}^{S} y_{ij} (t_j^{**} - t_i^{**}) \quad \text{(II-34)}$$

where t^* and t^{**} correspond to T^* and T^{**} and the summation is on all the points within and on the boundary and thus includes the boundary conditions. Because the Y matrix is a symmetric matrix, this finite sum has the symmetric relationship:

$$\sum_{i=1}^{S} t_i^* \sum_{j=1}^{S} y_{ij} (t_j^{**} - t_i^{**}) = \sum_{i=1}^{S} t_i^{**} \sum_{j=1}^{S} y_{ij} (t_j^{*} - t_i^{*}) \quad \text{(II-35)}$$

which is analogous to equation II-16. However, the use of A_i as a weighting factor here suggests that the best location for the points might be such that the weighting A_i is related to the weighting introduced by dV for the continuous case. The symmetric property of Y/A also can be shown in an indirect way by finding a symmetric matrix W that has the same negative eigenvalues of Y/A. This matrix, as found by expanding on arguments in Perlis (11), Theorem 9-13, is:

$$W = D\ Y\ D \tag{II-36}$$

where D is a diagonal matrix with $1/\sqrt{A_i}$ in the i^{th} diagonal position and the elements of W are:

$$w_{ii} = \mu_{ii} = -\frac{1}{A_i} \sum_{\substack{j=1 \\ i \neq j}}^{R} y_{ij} = \text{same diagonal element as } \frac{Y}{A}$$

$$w_{ij} = w_{ji} = \frac{y_{ij}}{\sqrt{A_i A_j}} = \mu_{ij} \frac{\sqrt{A_i}}{\sqrt{A_j}}$$

$$\mu_{ij} = \text{element of } \frac{Y}{A}$$

The algebraic approximation in equations II-31 and II-33 to the Laplacian could be used in other partial differential equations where the Laplacian occurs. For example, an approximate solution to Laplace's equation could be obtained by letting $\frac{d}{d\tau}(t) = 0$ in equation II-30 and solving the resulting system of algebraic equations.

The resulting system of linear ordinary differential equations are of an initial-value nature and may be solved analytically or on an analog computer. Also, any of the commonly used numerical integration methods could be used, such as one of Runge-Kutta's methods. The fourth-order Runge-Kutta method (12) in particular would give a very close approximation to the solution of the linear ordinary differential equations. However, this exact solution of the system of ordinary differential equations does not necessarily mean that a better approximation to the partial differential solution is obtained unless an extremely

fine space mesh is used, and thus the simple Euler's method or an implicit variation is usually used with adequate accuracy. This is true because, in the approximate solution of this partial differential equation of diffusion, the time-discretization error often compensates the space error and more accurate results are obtained. To formulate this procedure the temperature-time derivative is approximated by

$$\frac{d}{d\tau} t = \frac{1}{\Delta\tau}(t_{n+1} - t_n) \tag{II-37}$$

However, when this is substituted in equation II-31, a question arises whether the temperature vectors on the right side of equation II-31 should be evaluated at $n\Delta\tau$ or $(n+1)\Delta\tau$ or at an intermediate time. Assuming that a linear combination of vectors t_{n+1} and t_n is to be used, we may introduce weighting factors γ and $(1-\gamma)$. These factors are usually taken between zero and one, and are the weighting given to the temperature vector at $(n+1)\Delta\tau$ and $n\Delta\tau$, respectively. Thus, the temperature vector on the right hand side of equation II-31 is replaced with

$$t_{\tau_1} = (1-\gamma)t_n + \gamma t_{n+1} \tag{II-38}$$

$$n\Delta\tau \leq \tau_1 \leq (n+1)\Delta\tau$$

Introducing γ in our derived expressions gives not only the explicit forward-difference method when γ is zero, but also gives the implicit

type for γ not equal to zero; specifically, it gives central and backward differences when γ is $\frac{1}{2}$ or 1. More complicated methods of determining the vector $t_{\tau 1}$ for substitution on the right side of the difference equations have been suggested to improve the accuracy (6, 7) or the stability (5).

Continuing with the derivation, substituting $t_{\tau 1}$ for the temperature vector on the right side of equation II-31 and solving for t_{n+1}, we obtain

$$t_{n+1} = \left[I-\gamma\Delta\tau\frac{Y}{A}\right]^{-1}\left\{\Delta\tau\frac{Y_B}{A}(\gamma t_{B\,n+1}+[1-\gamma]t_{Bn})+\left[I+(1-\gamma)\Delta\tau\frac{Y}{A}\right]t_n\right\} \quad \text{(II-39)}$$

This equation is suitable for stepping out the approximate solution, although when γ is not zero a matrix inversion or equivalent operation is required. The solution of the equations for the implicit methods should not be considered a serious disadvantage, because the matrices usually contain many zeros, and are of a special form for which simplifications are possible (6). When $\gamma = 0$, the equation reduces to the explicit forward difference formulation used by Longwell (9) which requires no matrix inversion.

$$t_{n+1} = -\Delta\tau\frac{Y_B}{A}t_{B\,n}+\left[I+\Delta\tau\frac{Y}{A}\right]t_n \quad \text{(II-40)}$$

Here it should be strongly emphasized that these equations are those actually used in stepping out the numerical solution for successive time increments, starting with the known initial condition (t_0), and knowing how the boundary temperature changes with time.

There are several advantages to formulating the difference problem in this vector-matrix notation. The first is that this is a very general form that applies to one-, two-, or three-dimensional problems for an irregular, as well as a regular, distribution of points. Even though a specific set of rules, MacNeal's (8),was used in the derivation, using another system of rules would only change the elements in the Y/A matrix. As a matter of fact, Chapter V is a study of the accuracy of solutions using this matrix for an asymmetric distribution of nodes. Further, if a regular distribution of points is used, this formulation reduces to those represented by a partial difference equation. The second advantage is that for carrying out the calculations on a digital computer, matrix inversion, multiplication, and addition subroutines are generally available; consequently, the amount of programming necessary is greatly reduced. The third advantage is that a study of the vector-matrix equation itself gives a great deal of information concerning the usefulness, stability, and accuracy of the approximate method.

As mentioned above, for a regular location of the points the partial difference equation can be solved. This solution is found for the one-dimensional problem using z-transforms in Chapter IV. However, the formulation of the one-dimensional problem in matrix form is an example of the simplicity of this approach. In this case ℓ_{ij} becomes Δx for equally spaced points and r_{ij} is 1 for all i and j.

If the temperature vector is ordered either in increasing or decreasing subscripts m, the Y/A matrix is

$$\frac{Y}{A} = \frac{-1}{(\Delta\xi)^2} \begin{bmatrix} - & - & - & - & & - & - & - \\ -1 & 2 & -1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 & 0 & 0 \\ 0 & 0 & -1 & 2 & \cdots & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & \cdots & -1 & 2 & -1 \\ - & - & - & - & & - & - & - \end{bmatrix} \qquad \text{(II-41)}$$

The entries of the top and bottom rows are not specified since these entries are a direct result of the type of boundary conditions and the method used for approximation; these corresponding equations are derived from energy balances in Chapter IV, section B. The system of difference equations represented by the vector-matrix equation II-39 with Y/A matrix from equation II-41 can also be represented by the following partial difference equation, plus the two boundary condition equations.

$$-r\gamma t_{m-1,n+1} + (1+2r\gamma)t_{m,n+1} - r\gamma t_{m+1,n+1} = r(1-\gamma)t_{m-1,n} + (1-2r\{1-\gamma\})t_{m,n} + r(1-\gamma)t_{m+1,n} \qquad \text{(II-42)}$$

$m \neq$ subscripts for boundary points

$n = 0, 1, \ldots, \infty$

Usually the computational procedure is constructed from this partial difference equation. Note that only when the points are located in some regular manner is it possible to have a partial difference equation, and that generally, for any asymmetric arrangement, the elements of the Y/A matrix cannot be expressed by a simple recurrence formula.

This constitutes a general formulation for the numerical solution of the diffusion equation, which applies both to a regular and an irregular network of nodes. This was accomplished by treating the space differencing and the time differencing as separate problems. In addition to the diffusion equation a difference scheme for steady-state equations is also implied and analog approximations are also shown.

(D) SOLUTION OF APPROXIMATE FORMULATIONS

The main advantage of using difference methods for approximating the solution of partial differential equations is that the numerical results can be found without finding an analytic solution for the approximation. Thus, as previously pointed out, the system of algebraic equations II-39 or II-40 can be solved for successive time increments, stepping out an approximate solution, or the solution of a system of ordinary differential equations can be estimated using an electric analog. However, as the partial differential equation is actually just the special case of an approximate method that is consistent with the partial differential equation where the time and space increments are zero, and n and S are infinite, the approximate methods also have an analytic solution. In order to study both the stability and accuracy of an approximate method, a comparison between the form of the analytic solution for the approximate method and the form of the analytic solution of the partial differential equation is extremely useful. In the following discussion, the form of the solution for the system of difference equations is shown; analogies to the solution of the partial differential equation are indicated; and important properties and characteristics of the difference system are discussed and summarized for future reference. These results are not derived here, as they involve fairly long matrix arguments. Chapter III uses these solutions and

matrix properties to derive a rigorous but simple stability criterion. Chapter IV uses some of these results together with z-transforms to find analytic expressions for solutions using several approximate methods as applied to specific problems. Again, it should be emphasized that, although analytic solutions to the system of difference equations can be found, in order to study their behavior and the accuracy of the approximation, the way to find the numerical approximate solution is by using equation II-39.

The solution for the linear system of ordinary difference equations II-37 can be found by classical methods to be the sum of a particular and complementary solution. The solution vector is:

$$t_n = t_{P\,n} - C\,Q^n\,g \qquad \text{(II-43)}$$

where the i^{th} component of the vector is:

$$t_{i,n} = t_{P\,i,n} - \sum_{j=1}^{S} g_j\,c_{ij}\,q_j^n \qquad i = 1,\ 2,\ \ldots,\ S \qquad \text{(II-44)}$$

The particular solution $t_{P\,n}$ is an S-dimensional vector; it is found by the method of undetermined parameters or other methods, and it depends primarily on how the fluid temperatures in t_B, or forcing functions, change with space and time. This solution represents the steady-state solution if it does not change with time, or a quasi-steady-state if it is a function of time. The complementary solution $-C\,Q^n g$ is also an S-dimensional vector. It is the solution to the homogeneous system

of difference equations derived from equation II-39, which is:

$$\left[I - \gamma\Delta\tau\frac{Y}{A}\right]t_{n+1} - \left[I + (1-\gamma)\Delta\tau\frac{Y}{A}\right]t_n = 0 \qquad \text{(II-45)}$$

Both C and Q are S by S matrices and g is an S-dimensional vector. The matrix Q is a diagonal matrix with q_j in the j^{th} diagonal position. These S q_j's are the S real roots of the characteristic equation which is an S^{th} order polynomial.

$$\det\left[(q-1)I - (q\gamma + 1 - \gamma)\Delta\tau\frac{Y}{A}\right] = 0 \qquad \text{(II-46)}$$

The S q_j's are actually the eigenvalues of the matrix $[I-\gamma\Delta\tau(Y/A)]^{-1}[I+(1-\gamma)\Delta\tau(Y/A)]$. Since the matrix Q^n is the quantity in the approximate solution which corresponds to the damped exponential matrix $e^{-\upsilon^2\tau}$ in the continuous solution where the υ_j's are real, it can be seen that each q_j must be real, and between 0 and 1, to give the same type of behavior (or at least between -1 and +1 to be bounded); and the matrix arguments only show that the q_j's are real. Thus, to obtain a solution that is to be an approximation to the continuous solution we must select Y/A, $\Delta\tau$, and γ so that the q_j's meet this restriction; this is the topic of stability and is thoroughly discussed in Chapter III. However, for purposes of discussion, it will be assumed here that the q_j are all less than one in absolute value.

The j^{th} column of matrix C is the eigenvector of the matrix $[I-\gamma\Delta\tau(Y/A)]^{-1}[I+(1-\gamma)\Delta\tau(Y/A)]$ which corresponds to the j^{th} eigenvalue

q_j; it is defined by:

$$\left[(q_j-1)I - (q_j\gamma+1-\gamma)\Delta\tau \frac{Y}{A}\right]c_j = 0 \qquad j = 1, 2, \ldots, S \qquad \text{(II-47)}$$

The eigenvectors c_j are real and the set of S eigenvectors are linearly independent; the inverse of the eigenvector matrix C can be found explicitly, by using and expanding on matrix arguments in Perlis (11), Theorem 9-13, and using the relationship between Y/A and the symmetric W matrix, to be

$$C^{-1} = C'A \qquad \text{(II-48)}$$

where C' is the transpose of C. From this, the relationship analogous to the orthogonality relationship for the continuous solution is

$$\sum_{i=1}^{S} A_i c_{ij} c_{i\rho} = \delta_{j\rho} \qquad \rho, j = 1, 2, \ldots, S \qquad \text{(II-49)}$$

The vector g is found using the above inverse relationships so that the solution fits the initial condition:

$$g = -C'A (t_0 - t_{P\,0}) \qquad \text{(II-50)}$$

Its components are

$$g_j = -\sum_{i=1}^{S} A_i c_{ij} (t_{i,0} - t_{P\,i,0}) \qquad j = 1, \ldots, S \qquad \text{(II-51)}$$

The solution for the linear system of ordinary differential equations can be found either as the limiting case of the above solution as the time increment $\Delta\tau$ goes to zero, or directly from equation II-31 by classical methods. It is, in vector form:

$$t(\tau) = t_P(\tau) - C\, e^{\Lambda\tau}\, g \qquad \text{(II-52)}$$

where a component of $t(\tau)$ is

$$t_i(\tau) = t_{P\,i}(\tau) - \sum_{j=1}^{S} g_j\, c_{ij}\, e^{\lambda_j \tau} \qquad i = 1, 2, \ldots, S \qquad \text{(II-53)}$$

In this case the λ_j are the S negative real eigenvalues of the Y/A or W matrices, and are the S roots of the S^{th} order determinantal characteristic polynomial, which can be written in any of the following ways:

$$\det[\lambda I - \frac{Y}{A}] = \det[\lambda I - W] = [\det D]^2\, (\det[\lambda A - Y]) = 0 \qquad \text{(II-54)}$$

(each of the determinantal equalities are actually identical for all values of λ) where the roots are

$$\lambda_j < 0 \qquad j = 1, 2, \ldots, S \qquad \text{(II-55)}$$

In this case $(C\, e^{\Lambda\tau}\, g)$ does indeed represent a transient solution as the λ_j's are negative. Comparison of equations II-54 and II-46 gives us an important relationship between the eigenvalues of the Y/A matrix, λ_j, and of the difference system:

$$\lambda_j = \frac{q_j - 1}{(q_j + 1 - \gamma)\Delta\tau} \qquad j = 1, 2, \ldots, S \qquad \text{(II-56)}$$

or, solving for q_j:

$$q_j = \frac{1 + \lambda_j (1-\gamma)\Delta\tau}{1 - \lambda_j \gamma \Delta\tau} \qquad \text{(II-57)}$$

Also from equation II-47 and the relation between λ and q, equation II-56, and the fact that the Y/A matrix is not a function of the time increment, it is seen that the eigenvectors c_j can be taken as the eigenvectors of the Y/A matrix and are then the same for both the analog and difference approximations. Thus, if the particular solutions evaluated at time zero are the same for both the difference and analog approximations, as they are when the fluid temperatures are constant with time, the initial vectors are also identical. The particular solution represents the condition at infinite time for the analog solution, and it depends on how the boundary temperature changes with time.

(E) CONCLUSIONS AND SUMMARY

The transient temperature distribution in a solid, with a known initial temperature distribution and known boundary conditions, has been shown to be the continuous solution of a partial differential equation, the diffusion equation. This equation is derived by making an energy balance on a differential volume element, for a differential element of time, and it applies to the infinite points within the solid boundaries.

A difference approximation to the partial differential equation also has been presented. In this approximation a finite number of points is located within and on the solid boundaries, but not necessarily in a regular fashion. An energy balance based on a finite volume and a finite time increment for each point then gives a system of algebraic equations. By solving the algebraic equations for successive time increments, a numerical approximation of the transient temperature distribution can be stepped out, starting with the known initial conditions and using known forcing functions as a function of time.

Even though the points are not located regularly, the system of difference equations possesses several important properties that are analogous to properties of the partial differential equation. The matrix operator Y/A which replaces the Laplacian operator is negative definite, corresponding to the negative or stable character of the Laplacian. Although this matrix is not symmetric, it has a symmetric property

directly analogous to that of the Laplacian, and is similar to a symmetric matrix W. For the difference system, the negative and symmetric property is defined in terms of summations, which can be considered to be discretizations of the volume integrals which define the properties for the partial differential equation.

In addition to these analogies in the derivations and in the equations themselves, the system of difference equations has an analytic solution with the same form as the solution of the partial differential equation. The main advantage of the system of difference equations is that its solution can be stepped out numerically merely using algebraic techniques, but the analytic solution is not found in practice. However, a study of the form of the analytic approximate solution, and a comparison of it with the analytic continuous solution, are extremely important and useful in determining the stability criteria, and in analyzing the accuracy of an approximate method. As much of this thesis is concerned with an analysis of these solutions, it is appropriate to summarize and review here not only the analogies between the several parts of the solutions, but also to state which parts of both solutions are affected by changing the problem parameters, boundary conditions, and initial conditions, and which parts of the approximate solution are affected by changing the differencing parameters.

Both the continuous and difference solutions are made up of a transient solution and a particular solution (assuming stability of the

difference system). The particular solution governs the solution at long or infinite time and depends upon how the forcing functions change with time and the space variables. In general, if the forcing function is a constant, both particular solutions are constant; if the forcing function varies only with space variables, both particular solutions are functions of space variables; if the forcing functions are a function of time, the particular solutions are a function of space and time. In addition, the particular solution for the difference problem is affected by the discretization used for the variables upon which its particular solution depends. That is, for example, when the forcing function varies only with space variables, the approximate particular solution is also a function of the number and location of the points which fix the Y and Y_B matrices.

The transient solution of the continuous solution is an infinite sum of terms of the form $a_j b_j e^{-\nu_j 2_\tau}$ and of the difference solution is a finite sum of terms of the form $g_j c_j q_j^n$. In these solutions the exponential term $e^{-\nu_j 2_\tau}$ and the exponential form q_j^n correspond and determine the rate of change of the j^{th} term of the solution. Both the ν_j and the q_j are determined by a characteristic equation which depends upon the geometric and thermal properties of the solid and the boundary equations which are physical system variables. The eigenfunction b_j and eigenvector c_j determine the weighting of the j^{th} exponential (or exponential form) at each point where the solution applies. These

quantities are dependent upon the physical system variables. Although the eigenvectors c_j are not orthogonal vectors, according to the strict mathematical definition, a finite summation relationship exists that is directly analogous to the orthogonal integration of the eigenfunctions. The difference initial vector components g_j are found by fitting the initial condition with this finite summation relationship in the same way that the Fourier coefficients a_j are found with the orthogonal integration. These quantities then depend upon the initial temperature distribution and the nature of the particular solution, in addition to the physical system variables.

The difference transient solution also depends upon the space discretization parameters, the number and location of the points, and the time discretization parameters, the time increment and weighting γ. For the formulation in which the points are located and the equations calculated by MacNeal's rules, the Y/A and Y_B/A matrices are then fixed by the number and location of the points in addition to the properties of the physical system. Consequently, the eigenvectors c_j and eigenvalues λ_j depend upon the number and location of the points, but are independent of the time differencing parameters and of the forcing function or initial condition. The exponential forms q_j^n depend upon both the time differencing parameters $\Delta\tau$ and γ, in addition to the space differencing, as it affects λ_j. For forcing functions that are constant, or a function only of space, the only differencing parameter that affects

the g_j is the number and location of points. If the particular solution evaluated at zero is a function of the time differencing, then the g_j's also depend upon the time differencing.

Because of the additional dependence of the approximate solution on the differencing parameters, nothing can be inferred about the accuracy of the approximate solution. As mentioned previously, we are not even assured of the stability of the difference system. A useful stability criterion is developed in the next chapter, and accuracy is discussed in the final two chapters.