CHAPTER IV

SOLUTIONS OF THE ONE-DIMENSIONAL PARTIAL DIFFERENCE EQUATION FOR DIFFUSION IN CARTESIAN COORDINATES USING z-TRANSFORMS

(A) INTRODUCTION

In this chapter a z-transform method is presented for finding the complete analytic solution of linear partial difference equations of an initial-value type. This method is then used to find the solution of the partial difference equation II-42 which approximates the one-dimensional diffusion equation in Cartesian coordinates for several methods of approximating typical initial and boundary conditions. A comparison of the analytic difference and continuous solutions is then made.

The discussion in Chapter II has shown the solutions to the continuous partial differential equation and the difference formulation to be in the same form. A useful criterion has been derived in Chapter III for selecting the time differencing parameters so that the transient difference solution must have a behavior like that of the transient continuous solution. However, no mention was made of accuracy, or how well the difference eigenvectors, eigenvalues, initial vector, and particular

solution approximate the corresponding continuous eigenfunctions, eigenvalues, initial vector, and particular solution, or how well the total expression approximates the continuous expression. One way of making this comparison is to numerically step out an approximate solution for a problem where the continuous solution is known, and then compare the calculated continuous solution with the stepped-out approximate solution. Although this method of comparison does give results that show the accuracy for the specific problem with specific mesh size and other approximations and which reflect the accuracy and interrelationships between the various quantities mentioned above, it does not give any understanding or insight as to why the approximate method behaved as it did. Further generalizations made from such a comparison might be questionable. As a matter of fact, such a comparison of two possible graphical methods, for the case of specified boundary conditions, initially stimulated the search for a way to find the complete analytic difference solution or analytic expressions for all the quantities shown in equation II-43.

The specific problem that initiated this study was a comparison between graphical methods C and G for a specified boundary temperature. (Details of these methods are discussed later.) The results for a calculation of the temperature of the point nearest the boundary versus dimensionless time are shown in Figure IV-1 along with the continuous solution. The results for graphical method C oscillate so badly that

while the solution is stable it is useless; graphical method G on the other hand gives results which, although oscillatory, are useful. These results would not be anticipated as the norms of the Y/A matrix for both methods were equal and, further, a preliminary calculation of the eigenvalues for each method for two by two and three by three matrices indicated that both methods had identical eigenvalues. The complete solution not only explains this behavior, but it gives a much better understanding of the methods, shows ways of improving them, and allows us to make valid generalizations.

As demonstrated in Chapter II, for a regular mesh the approximate formulation for the one-dimensional diffusion equation in Cartesian coordinates can be shown as a partial difference equation, equation II-42, or by the matrix vector equation II-39, where the Y/A matrix is in equation II-41. In that matrix, the top and bottom rows are not shown. In the next section two general derivations for these equations are given which are approximations to the continuous boundary condition equation:

$$\pm h\left[T_f(\tau) - T(\xi_b \tau) \right] = \frac{k}{L} \frac{\partial T}{\partial \xi}(\xi_b \tau) \qquad \text{(IV-1)}$$

From the resulting general equations, several generalized methods are defined based on the selection of the formulation parameters that correspond to graphical methods A, C, G, and F (20). Although these define the calculation procedure, modifications are sometimes used

such as averaging, interpolating, and using slightly different initial temperatures and/or fluid temperatures, other than those directly suggested by the continuous problem. Specification of the calculation procedure and the modifications to the boundary and initial temperature functions then complete the difference formulation as a partial difference equation, subject to two boundary conditions and an initial distribution. Its solution is unique.

Next the z-transforms are defined from Laplace transforms and their important properties derived. Several related example problems are solved for approximate method G. These solutions show that the z-transform procedure is exactly analogous to the Laplace transform procedure for partial differential equations. The partial difference equation and its boundary equations are transformed. The resulting boundary-value ordinary difference equation is solved. The transformed temperature is then inverted to find the complete analytic expression for the difference solution which fits the initial and boundary conditions and includes the particular solution. Further, this solution is in a form that can be directly compared with the continuous solution.

This method gives the complete solution directly, in contrast to the classical methods of direct attack on matrix eigenvalue-eigenvector problems and the separation of variables or substitution technique suggested by von Neumann, as quoted in references (2, 21). The analytic solution for matrix eigenvalues is possible using the work of

Wolstonholne as quoted in Muir (22) and extended by Rutherford (23, 24). This is based on simple yet sophisticated use of a determinantal equation like equation II-46. A difficult analysis is required to determine the eigenvectors. Further, it is only applicable when the Y/A matrix is symmetric, so method G could not be studied in this way. The results have been used by Todd (4) for an approximation to the problem where the boundary temperature is specified. The technique of von Neumann is directly analogous to the separation of variables technique for solution of partial differential equations, and this method is usually used to derive the stability criteria for cases where a boundary temperature is specified (10, 21, 17, 15, 2, 18). The eigenvectors and eigenvalues are obtained directly upon fitting the boundary equations.

Although both the separation of variables technique and the matrix methods could be used for cases of finite non-zero heat-transfer coefficient, no references have been found where this has been done. Also, after the eigenvectors and eigenvalues have been found, to obtain the complete solution the particular solution must be determined and the coefficients required to make the solution fit the initial conditions must be found. This determination of the initial vector requires finding and using the orthogonal relationships of the eigenvectors, equations II-49 and II-51, and the analytic evaluation of several finite sums, essentially a finite harmonic or Fourier analysis. Only for one

approximation in the case of the infinite heat-transfer coefficient is this complete solution reported (2). These finite Fourier coefficients or the initial vector have an important effect on the accuracy of an approximate solution.

The last section of this chapter presents a comparison of the analytic expression of the solutions for the difference methods mentioned for several problems with the continuous solution of these problems (each of the defined methods is not necessarily derived or compared for each problem). These problems for the comparison are usually taken with a zero initial condition for convenience and they are summarized in Table IV-9.

(B) DIFFERENCE FORMULATION

In the formulation of the difference equations in Chapter II, the equations for interior points were fully developed from MacNeal's rules for both regular and irregular distributions of temperature points. No mention was made specifically (except by implication) of how the boundary conductances for cases of finite heat-transfer coefficient would be calculated or what assumptions could be made about the heat capacity of the boundary points. However, Longwell (20) has used a method for finite heat-transfer coefficient in association with his numerical solutions using an asymmetrical network. Also, he and his co-workers have pointed out that several different approximations to the boundary conditions may be used for graphical solutions for one-dimensional problems which give different results (20).

Here, the difference equations which approximate boundary conditions are derived in a general fashion for the one-dimensional problem for a node on the surface or $\Delta\xi/2$ inside the surface. These are the equations that would give the top and bottom rows in the Y/A matrix in equation II-41. For the point locations shown in Figures IV-2 and IV-3, the derivations are made in such a way that generalizations of the more accurate graphical methods mentioned in the references are obtained. This then completes the Y/A matrix for the one-dimensional problem.

If the initial temperature distribution, $t_{m,0}$, and the fluid temperature, $t_{f,n}$, are found directly from the corresponding continuous conditions, the method is specified. However, for more accuracy the initial temperature distribution and/or the fluid temperature function to be used in the approximate calculation are often modified slightly from the continuous conditions. Averaging or interpolation of the approximate results is also used sometimes. Thus, to completely specify a method, not only the grid and calculation equations must be specified, but also whether and how the initial temperature distribution and fluid temperature functions are to be modified, and if interpolation or averaging is to be used. In this study, the general equations are derived for each of the two meshes first. From these derivations certain logical assumptions follow concerning the initial conditions. Next, averaged methods are defined which can be applied to the methods. These averaged methods are shown to give the identical results as interpolation in some cases, and as certain modifications to the initial distribution and/or the fluid temperature function.

1. Continuous Problem and Initial Condition

The problem to be approximated in one dimension is

$$\frac{\partial T}{\partial \tau} = \frac{\partial^2 T}{\partial \xi^2} \qquad 0 < \xi < 1 \qquad \tau > 0 \qquad \text{(IV-2)}$$

with the known initial condition

$$T = T(\xi, 0) \qquad 0 < \xi < 1 \qquad \tau = 0 \qquad \text{(IV-3)}$$

and the two boundary conditions found by energy balances on the surface

$$H_0 \left[T_{f_0}(\tau) - T(0,\tau) \right] = -\frac{\partial T}{\partial \xi}(0,\tau) \qquad \xi = 0 \qquad \tau \geq 0 \qquad \text{(IV-4)}$$

$$H_L \left[T_{f_L}(\tau) - T(1,\tau) \right] = +\frac{\partial T}{\partial \xi}(1,\tau) \qquad \xi = 1 \qquad \tau \geq 0 \qquad \text{(IV-5)}$$

$$0 \leq H \leq \infty$$

where $H = hL/k$ = dimensionless heat-transfer coefficient

$T_f(\tau)$ = known function of time

The above initial condition, as specified, might not be known at the boundaries and in using an approximate solution with a point on the boundary, one must use a temperature for the boundary point to start the calculation. For this reason a brief discussion of the initial distribution follows. First, the exact continuous solution evaluated at time zero fits the boundary conditions, equations IV-4 and IV-5, evaluated at time zero. This means that, for the case of an infinite heat-transfer coefficient or specified boundary temperature initially, the boundary temperature does not equal the initial distribution found by extending equation IV-3 to the boundary. Two initial distributions can then be defined which apply for all ξ, including the boundaries. The first is designated $T(\xi, 0+)$ which results from the Fourier series for the continuous solution evaluated at a time of zero. It can be considered to be

the temperature distribution the instant after the boundary conditions are imposed. In most cases, this is known even if the exact solution is not. If h is less than infinity, then no discontinuity occurs at the boundary; this can be seen from Laplace transforms. If h is infinity, then the boundary temperature is equal to the fluid temperature. In some cases, either because of the method being used, or because $T(\xi, 0+)$ is not obvious, a second distribution is designated as $T(\xi, 0-)$ and is the distribution for the interior extended to the boundary. It can be considered the temperature distribution the instant before the boundary conditions are applied. For a finite heat-transfer coefficient it is the same as $T(\xi, 0+)$; for infinite heat-transfer coefficient initially the surface temperature would not be the fluid temperature, but would be the temperature of the material an infinitesimal distance inside the surface.

2. Meshes

The regular difference meshes that may be used for the one-dimensional diffusion equation are in Figures IV-2 and IV-3. A point which has two points as neighbors located $\pm\Delta\xi$ from it is called an interior point. The other points, which are located on or adjacent to a boundary with a conductance to a known fluid temperature, or with a known heat flux input, are called adjacent nodes. The main difference between the four meshes is that, in some cases, an adjacent node is

located on the boundary while in other cases it is located at a distance of $\Delta\xi/2$ from the boundary. Only the meshes with both boundary points located on the boundary or at a distance $\Delta\xi/2$ inside, as shown in Figure IV-2, are studied here.

The partial difference equation for diffusion in one dimension for the m^{th} interior point as derived from Taylor expansions or Mac-Neal's rules is

$$\frac{t_{m,n+1} - t_{m,n}}{\Delta\tau} =$$

$$\frac{1}{(\Delta\xi)^2}\left[\gamma\left\{t_{m-1,n+1} - 2t_{m,n+1} + t_{m+1,n+1}\right\} + (1-\gamma)\left\{t_{m-1,n} - 2t_{m,n} + t_{m+1,n}\right\}\right]$$

$$1 \le m \le S-1 \qquad \text{(IV-6)}$$

Rearranging this equation gives equation II-42 and defines all but two rows of the Y/A matrix. In mesh $\Delta\xi$, Figure IV-2, this equation is written for $m = 1, 2, \ldots, S$; for mesh $\Delta\xi/2$ in Figure IV-2, it is written for $m = 3/2, 5/2, \ldots, S-3/2$. It serves to define all but the upper and lower rows of the Y/A matrix in equation II-33, where the two equations for the adjacent points are not given.

To derive the boundary equations, an energy balance at an adjacent point is solved for the temperature at that point. We will do this for both the $\Delta\xi$ and $\Delta\xi/2$ type adjacent points, and for the left adjacent point ($\xi = 0$ or $\xi = 1/2S$); the result can easily be applied to the opposite end. The derivations made are sufficiently general to obtain

a generalization of the graphical methods, including Longwell's backward difference type approximation (graphical method A), in addition to a general implicit formulation.

3. Mesh $\Delta\xi$

First consider mesh $\Delta\xi$ and the point 0. The energy in from a fluid is

$$h(t_f - t_0) = \dot{q}_{in} \tag{IV-7}$$

and out is

$$\frac{k(t_0 - t_1)}{L\,\Delta\xi} = \dot{q}_{out} \tag{IV-8}$$

Assuming an area associated with this point as $(\Delta\xi/2)$ we may write the accumulation term as

$$\sigma C_p \frac{L\,\Delta\xi}{2}\left[\frac{t_{0,n+1} - t_{0,n}}{L^2\Delta\tau/K}\right] = \text{volume rate of accumulation} \tag{IV-9}$$

Now the problem again occurs as to when to take the energy in, $\dot{q}_{in}$, and out, $\dot{q}_{out}$. Two weighting factors are defined, β and φ, such that β, $(1-\beta)$, φ, and $(1-\varphi)$ lie between zero and one. The weighting β is given to the energy in from the surrounding fluid at time $(n+1)$, and $(1-\beta)$ to that quantity at time n. Analogously, φ is the weighting given to the energy out from the interior node at time $(n+1)$, and $(1-\varphi)$ at time n. The energy balance then becomes (in dimensionless variables)

$$\frac{\sigma C_p L \Delta\xi}{2} \quad \frac{t_{0,n+1} - t_{0,n}}{\sigma C_p L^2 \Delta\tau / k} = h\left[(t_{f,n+1} - t_{0,n+1})\beta + (t_{f,n} - t_{0,n})(1-\beta)\right] \tag{IV-10}$$

$$- \frac{k}{L\Delta\xi}\left[(t_{0,n+1} - t_{1,n+1})\varphi + (t_{0,n} - t_{1,n})(1-\varphi)\right.$$

(If h is not constant it should be included in the β weighting.)

Combining and rearranging so that unknown temperatures at (n+1) are on the left side of the equation, the calculation equation for the adjacent point is:

$$t_{0,n+1}\left[1 + 2r\left(\frac{H\beta}{S} + \varphi\right)\right] - 2r\varphi t_{1,n+1} = t_{0,n}\left[1 - 2r\left\{\frac{H}{S}(1-\beta) + 1 - \varphi\right\}\right]$$

$$+ t_{1,n}\left[2r(1-\varphi)\right] \tag{IV-11}$$

$$+ \frac{2rH}{S}\left[t_{f,n+1}\beta + (1-\beta)t_{f,n}\right]$$

where $\Delta\xi = 1/S$

and $r = \Delta\tau/(\Delta\xi)^2$

Using a similar boundary equation for $t_{S,n+1}$ then specifies the calculation procedure, but does not specify the initial distribution or how the boundary temperature changes with time. This equation is convenient for all H less than infinity. By taking limits as H goes to infinity, which means neglecting the capacity of the surface node, the boundary condition equation for a specified boundary temperature is:

$$(t_{0,n+1} - t_{f,n+1})\beta = (1-\beta)(t_{f,n} - t_{0,n}) \qquad n \geq 0 \qquad \text{(IV-12)}$$

If β is not one and the above expression is to hold for all n, it is necessary in order to avoid oscillations that

$$t_{f,0} = t_{0,0} \qquad \text{(IV-13)}$$

otherwise a root q_j of $(\beta-1)/\beta$ would be added to the transient solution. For $\beta = 1$ the initial conditions $t_{0,0}$ need not be equal to $t_{f,0}$ as equation IV-10 gives

$$t_{0,n+1} = t_{f,n+1} \qquad n \geq 0 \qquad \text{(IV-14)}$$

In this case $T(m\Delta\xi, 0-)$ is used as the difference initial condition.

Two specific methods of the many defined by equation IV-10, and which are to be studied, are generalized methods A and G. These methods are defined only for mesh $\Delta\xi$; thus the equations for both boundary equations are defined by equation IV-11 where a different H_S and $t_{f_S,n}$ and different subscripts define the right hand ($\xi = 1$) boundary condition.

Method G. First method G is defined and derived. For this method, β and φ in the boundary equations are set equal to γ in the partial difference equation IV-6. This gives for the left boundary:

$$t_{0,n+1}\left[1 + 2r\gamma\left(\frac{H}{S} + 1\right)\right] - 2r\gamma t_{1,n+1} = t_{0,n}\left[1 - 2r(1-\gamma)\left(\frac{H}{S} + 1\right)\right] + 2rt_{1,n} + \frac{2rH}{S}\left[t_{f,n+1}\gamma + t_{f,n}(1-\gamma)\right] \qquad \text{(IV-15)}$$

This is a generalization of the implicit case of Longwell's (9) approximation for finite heat-transfer coefficient and it gives a Y/A matrix with all the properties described in Chapter II. However, this method suffers from a serious defect. The sufficient stability criterion from an examination of the Y/A matrix for all H less than infinity is

$$r(1 - 2r\gamma)M < 2 \tag{IV-16}$$

$$\text{where } M = \min \left(\left\| \frac{Y}{A} \right\|_{I}, \left\| \frac{Y}{A} \right\|_{II} \right) \tag{IV-17}$$

$$\left\| \frac{Y}{A} \right\|_{I} = 2\left(2 + \frac{H_{MAX}}{S}\right)$$

$$\text{and} \tag{IV-18}$$

$$\left\| \frac{Y}{A} \right\|_{II} = \text{MAX}\left(5 \text{ or } 3 + \frac{H_{MAX}}{S}\right)$$

This means that for an explicit method and a non-zero H a more severe restriction than r less than one-half must be used. One way to reduce this limit would be to neglect the capacity of the surface node $LC_p\sigma\Delta\xi/2$; (this is essentially what is done when H is increased to infinity) and the temperature at the surface is then for any time increment an explicit function of $t_{f,n}$ and $t_{1,n}$ at the same value of n.

$$t_{0,n} = \frac{\frac{H}{S} t_{f,n} + t_{1,n}}{\frac{H}{S} + 1} \tag{IV-19}$$

This equation can then be used to eliminate $t_{0,n}$ from the partial difference equation written for an m of 1. Thus, $t_{0,n}$ need not be computed; the Y/A matrix is reduced by one row and one column and the largest eigenvalue of Y/A is eliminated. However, as method G is defined, only for the case of a specified boundary temperature (infinite h) is the capacity of node 0 neglected. This method normally uses $T(m\Delta\xi, 0+)$ for its initial condition and $T_f(n\Delta\tau)$ for the difference fluid temperature. The details of this method are summarized in Table IV-1.

Method A. To avoid instability with a large, but finite, heat-transfer coefficient, Longwell (20) has suggested using a backward difference approximation for the energy into the solid at the surface, for a graphical method. A generalization of this principle is seen from the above equation IV-11; for if φ is zero an explicit equation for $t_{0,n+1}$ results.

$$t_{0,n+1} = \frac{t_{0,n}\left[1-2r\left\{\frac{H}{S}(1-\beta)+1\right\}\right] + 2rt_{1,n} + \frac{2rH}{S}\left[t_{f,n+1}\,\beta + t_{f,n}(1-\beta)\right]}{\left[1 + 2r\,\frac{H\beta}{S}\right]} \qquad \text{(IV-20)}$$

Although using an equation of the form of equation IV-20 for each boundary and using a non-zero γ in the partial difference equation is in principle possible, the main advantage of using the backward difference is to have a stable explicit method where the heat capacity of the

surface node is not neglected. In this explicit case, the Y/A matrix is not defined directly, but since $[I - Y/A]$ is defined as the matrix that operates on t_n, an equivalent Y/A may be found by difference. The first few rows are:

$$(\Delta\xi)^2 \frac{Y}{A} = - \begin{vmatrix} \frac{2(\frac{H}{S} + 1)}{1 + 2r\frac{H\beta}{S}} & - \frac{2}{1 + 2r\frac{H\beta}{S}} & 0 \ \ldots \\ -1 & 2 & -1 \ \ldots \\ \cdot & \cdot & \\ \cdot & \cdot & \\ \cdot & \cdot & \end{vmatrix} \qquad \text{(IV-21)}$$

From the norms, the sufficient stability criteria are

$$r\left[\frac{H}{S}(1 - 2\beta) + 2\right] \leq 1 \qquad \text{(IV-22)}$$

and $$r \leq \tfrac{1}{2} \qquad \text{(IV-23)}$$

If β is equal to or greater than $\frac{1}{2}$ the second inequality is the more restrictive, thus avoiding the much more restrictive stability requirement in equation IV-16. Although the Y/A matrix must be found by difference for the above family of methods where φ and γ are zero, but not equal to β which is not zero, the resulting Y/A matrix retains all the properties mentioned in Chapter II, except that it is now also a function of the time increment $\Delta\tau$ or r. This is in contrast to method

G where the Y/A matrix has all the properties described in Chapter II and is not a function of the time differencing parameters.

Longwell (19) has shown the advantageousness of a graphical method A based on equation IV-20 with a β of 1 and an r of $\frac{1}{2}$. In this study, a generalized method A is defined on the same equation with a β of 1 but for all r that give stable solutions. The boundary equation is

$$t_{0,n+1} = \frac{t_{0,n}(1-2r) + 2r\, t_{1,n} + \frac{2r\, H_0}{S}\, t_{f_0,n+1}}{1 + 2r\, \frac{H_0}{S}} \qquad \text{(IV-24)}$$

Note that if H is not constant its value should be taken at the end of the time increment. This equation is used to calculate the boundary temperature for all finite H. If H is zero, it reduces to the same equation as explicit method G. For infinite H, taking limits gives directly,

$$t_{0,n+1} = t_{f,n+1} \qquad n \geq 0 \qquad \text{(IV-25)}$$

The difference initial distribution for this method is taken as $T(m\Delta\xi, 0-)$ for all n including the points on the surface. Thus for infinite h the surface temperature point does not change until an n of one is reached. Then this method results in delaying the change in $t_{0,n}$ only for the first time increment. For problem II where one surface temperature is constant, the other adiabatic, an implicit method A is defined, which

gives the same results as implicit G, but delayed one time increment. However, for all other problems method A is an explicit method. Details of this method are summarized in Table IV-2.

4. Mesh $\Delta\xi/2$

Next consider mesh $\Delta\xi/2$ where there are no points on the boundary, but a boundary point is located a distance of $\Delta\xi/2$ in from the surface. An energy balance is made on the left adjacent node, $\frac{1}{2}$. The energy rates in and out are:

$$\dot{q}_{in} = \frac{t_f - t_{\frac{1}{2}}}{\frac{1}{h} + \frac{\Delta x/2}{k}} = \frac{h(t_f - t_{\frac{1}{2}})}{1 + \frac{H}{2S}} \qquad \text{(IV-26)}$$

$$\dot{q}_{out} = \frac{k(t_{\frac{1}{2}} - t_{3/2})}{\Delta x} = \frac{k(t_{\frac{1}{2}} - t_{3/2})}{L\Delta\xi} \qquad \text{(IV-27)}$$

and the rate of accumulation is:

$$\text{rate of accumulation} = L\Delta\xi\sigma C_p \left[\frac{t_{\frac{1}{2},n+1} - t_{\frac{1}{2},n}}{L^2\sigma C_p \Delta\tau/k} \right] \qquad \text{(IV-28)}$$

Again using β and $(1-\beta)$ for the energy from the fluid and φ and $(1-\varphi)$ for the energy to the adjacent interior point the energy balance gives

$$t_{\frac{1}{2},n+1}\left[1+r\,\frac{\beta\,H/S}{1+H/2S}\right]-r\varphi t_{3/2,n+1}=t_{\frac{1}{2},n}\left[1-r\left\{\frac{(1-\beta)H/S}{1+H/2S}+1-\varphi\right\}\right]$$

$$+r(1-\varphi)t_{3/2,n}+\left[\frac{r\,H/S}{1+H/2S}\right]\left[(1-\beta)t_{f,n}+\beta t_{f,n+1}\right] \qquad \text{(IV-29)}$$

This equation is suitable for use for all H less than infinity. Taking limits as H goes to infinity, which does not require neglecting any heat capacity, gives

$$t_{\frac{1}{2},n+1}[1+r(2\beta+\varphi)]+r\varphi t_{3/2,n+1}=t_{\frac{1}{2},n}[1-r\{2(1-\beta)+1-\varphi\}]$$

$$r(1-\varphi)t_{3/2,n}+2r[(1-\beta)t_{f,n}+\beta t_{f,n+1}] \qquad \text{(IV-30)}$$

These equations and the derivations are somewhat unique in that no temperature point is located on the boundary. If it is necessary to compute a surface temperature, one may do so using thermal resistances, and no thermal capacity associated with the surface point.

$$t^{*}_{n}=\frac{t_{\frac{1}{2},n}+\frac{H}{2S}t_{f,n}}{1+\frac{H}{2S}} \qquad \text{(IV-31)}$$

where t^{*}_{n} = surface temperature at n ($t_{0,n}$ is not used, as m is restricted to full increments; also, the difference solution does not give this temperature by letting m = 0 for this mesh)

or, rearranged,

$$H\left[t_{f,n} - t^{*}_{n}\right] = \frac{(t^{*}_{n} - t_{\frac{1}{2},n})}{\Delta\xi/2} \qquad \text{(IV-32)}$$

which is a direct difference approximation of the continuous boundary condition, equation IV-4. In several other ways, mesh $\Delta\xi/2$ leads to approximations that appear to be closer mathematically to the continuous problem than does mesh $\Delta\xi$. First of all, as each node has the same thermal capacity, the Y/A matrix is symmetric for all values of H when β and φ are taken equal to γ. In this case, its eigenvectors are orthogonal with respect to a weighting factor of one as the eigenfunctions of the continuous solution are orthogonal with respect to a weighting factor of one. Moreover, even for infinite h no heat capacity is neglected. Further, as no point is selected on the surface, the initial condition need not be specified on the surface, as is also the case for the continuous problem.

Method C. First, method C is defined which is analogous to method G in that β and φ are taken equal to γ in the partial difference equation. The boundary equations for finite and infinite H are, respectively,

$$t_{\frac{1}{2},n+1}\left[1+r\gamma\left(\frac{1+3H/2S}{1+H/2S}\right)\right] - r\gamma t_{3/2,n+1} = t_{\frac{1}{2},n}\left[1-r(1-\gamma)\left(\frac{1+3H/2S}{1+H/2S}\right)\right] \qquad \text{(IV-33)}$$

$$+ r(1-\gamma)t_{3/2,n} + \left[\frac{rH/S}{1+H/2S}\right]\left[(1-\gamma)t_{f,n} + t_{f,n+1}\right]$$

$$t_{\frac{1}{2},n+1}(1+3r\gamma) - r\gamma t_{\frac{1}{2},n+1} = t_{3/2,n}[1-3r(1-\gamma)]$$
$$+r(1-\gamma)t_{\frac{1}{2},n} + \left[(1-\gamma)t_{f,n} + \gamma t_{f,n+1}\right] \qquad \text{(IV-34)}$$

The Y/A matrix for this method has all the properties described in Chapter II and from its norms method C is stable for

$$r(1 - 2\gamma) \leq \tfrac{1}{2} \qquad \text{(IV-35)}$$

Graphical method C reduces to Schmidt's graphical method, as given in reference (19), except that his calculation for an n of zero does not follow equation IV-32 but does follow a construction for finite h that gives a t_0 that corresponds to the continuous surface temperature initially (note equation IV-31 does change the surface temperature for an n of zero). Also, although the graphical method is technically stable for all H, it is not used for cases where H/S is greater than 2, because of large oscillations. Details of method C are summarized in Table IV-3.

Method F. In order to avoid these oscillations for infinite h Schmidt proposed an alternate construction, called method F in the Longwell manuscript (20), for infinite h only. If in equation IV-31 we let $\beta = \frac{1}{2}$, $\varphi = 0$, $r = \frac{1}{2}$, and $\gamma = 0$, for the case of a constant fluid temperature the equation reduces to Schmidt's construction. Thus a generalized explicit method F may be defined by making $\beta = \frac{1}{2}$ and φ and γ zero. Details of this generalized method are in Table IV-4; however, here only the graphical method for infinite h is studied.

5. Other Methods

Although these are the basic four methods studied here, two other methods probably should be investigated. These are an explicit method for mesh $\Delta\xi$ with a β of $\frac{1}{2}$ and an explicit method for mesh $\Delta\xi/2$ with a β of 1. Also combination methods for the meshes shown in Figure IV-3 could be studied.

6. Graphical Solution

The system of difference equations given by the partial difference equation IV-6 and the boundary equations for one of the methods, G, A, C, or F, can usually be solved by a graphical construction when the differencing parameters are selected by

$$r = S^2\Delta\tau = \tfrac{1}{2} \qquad \text{(IV-36)}$$

$$\gamma = 0 \qquad \text{(IV-37)}$$

The simple graphical constructions for both the interior points and the boundary equations are described in the study by Longwell (20). However, simple graphical constructions that solve the boundary equations for methods G and F for H's that are neither zero nor infinite are not available. (Also method G is unstable for these H's and the combination of differencing parameters given in equations IV-36 and IV-37.) However, the selection of the r and γ according to equations IV-36 and IV-37 is important, even if the solution is calculated numerically rather than graphically. This is true because under these conditions

the number of non-zero multiplications required per step is S compared to 2S for any other explicit calculation ($\gamma = 0$) or 7S for an implicit calculation ($\gamma \neq 0$). This comparison of calculation counts assumes that advantage is taken of the fact that the off-diagonal elements in each row of the $[I-(1-\gamma)\Delta\tau(Y/A)]$ matrix are equal, and that use is made of the elimination method of solving the equations for an implicit calculation, as described in Chapter III. If a general vector-matrix multiplication is used to calculate $\left[I-(1-\gamma)\Delta\tau\left(\frac{Y}{A}\right)\right]t_n$, S multiplications must be added to each number giving 2S for graphical, 3S for explicit, and 8S for implicit calculations. Because of the ease of stepping out the solution either graphically or numerically a special designation is used for the solution when γ is zero and r is $\frac{1}{2}$. Since either the graphical or numerical stepping out of the solution in the absence of errors gives the same approximation, in this study selection of the parameters according to equations IV-36 and IV-37 for any method is called a graphical solution or graphical method. If the number of points to be used is greater than about eight, the graphical construction to step out the solution becomes inaccurate and the approximate solution must be stepped out numerically.

The general definition of graphical methods together with specific notes on the graphical solutions associated with each method is in Table IV-5. For more details concerning construction and a comparison of numerical results for specific problems the Longwell (20) reference

should be consulted.

7. Averaged Methods

Although the equations presented for each method, together with a straightforward use of the initial temperature distribution and the forcing functions, serve to completely define an approximate method, several modifications can be applied to these methods without changing the equations or matrix elements. In this section, the technique of averaging the approximate solution as mentioned in Chapter III is more fully defined and discussed. The important relationship between an averaged method and an unaveraged method is developed. Also brief sections are included on interpolation as suggested by Longwell (20) and on the modification of the fluid temperature function for step changes in fluid temperature. In these sections these techniques are defined and they are shown to be equivalent to an averaging procedure. Then, based on these equivalences, a specific averaged method is associated with the equations for methods G, A, C, and F.

In an averaged method the approximate solution of one of the defined methods is stepped out according to equation II-39 in the usual manner. The temperature vector t_n found for the beginning of the $(n+1)$ time increment and t_{n+1} for the end of that time increment are averaged and assumed to apply at the beginning, at the end, or at some time within the $(n+1)$ time increment. The defining equation for the averaged temperature vector $t_{n+k\ Ave}$ assumed to apply at time $(n+k)\Delta\tau$

is:

$$t_{n+k\,Ave} = \tfrac{1}{2}\,(t_n + t_{n+1}) \qquad \text{(IV-38)}$$

where t_n and t_{n+1} are the unaveraged temperature vectors found by successive uses of equation II-39. The parameter k is analogous to the weighting factor γ and tells at what fraction of the time increment the average applies; it is taken between zero and one inclusive:

$$0 \le k \le 1 \qquad \text{(IV-39)}$$

In this study k is usually 0 or 1, although a brief study of a k of $\frac{1}{2}$ is also made. For a k of zero, the average is called a forward average because it is analogous to the forward difference calculation when the weighting factor γ is zero as both involve t_{n+1} in the calculation at time n.

Forward Average, k = 0:

$$t_{n\,Ave} = \tfrac{1}{2}\,(t_n + t_{n+1}) \qquad n \ge 0 \qquad \text{(IV-40)}$$

Likewise the central and backward averages are defined by

Central Average, $k = \frac{1}{2}$:

$$t_{n+\frac{1}{2}} = \tfrac{1}{2}\,(t_n + t_{n+1}) \qquad n \ge 0 \qquad \text{(IV-41)}$$

Backward Average, k = 1:

$$t_{n+1\,Ave} = \tfrac{1}{2}\,(t_n + t_{n+1}) \qquad n \ge 0 \qquad \text{(IV-42)}$$

The backward average can be written for time n for convenience in comparing with the forward average as:

Backward Average, k = 1:

$$t_{n\,Ave} = \tfrac{1}{2}\left(t_{n-1} + t_n\right) \qquad n \geq 1 \qquad \text{(IV-43)}$$

Of these averages only the forward average can be used to calculate a temperature vector at a time of zero, and hence only the forward average (or only when k is zero) can change the initial temperature distribution.

Although the averaging technique is defined as averaging the approximate solution vectors for successive times n and (n+1) as calculated directly from the stepping out of equation II-39, identical results can be obtained by using an averaged temperature vector $t_{n+k\,Ave}$ and an averaged boundary temperature vector $t_{B\,Ave}$ in equation II-39 to step out the solution. This can be proved by writing equation II-39 for t_{n+1} in terms of t_n and t_{n+2} in terms of t_{n+1} and substituting these quantities in equation IV-38 which defines an averaged method. This gives, using the definition of $t_{n+k\,Ave}$:

$$t_{n+k+1\,Ave} =$$

$$\left[I-\Delta\tau\frac{Y}{A}\right]^{-1}\left(\left[I+(1-\gamma)\Delta\tau\frac{Y}{A}\right]t_{n+k\,Ave}+\Delta\tau\frac{Y_B}{A}\left[\gamma t_{B\,n+2}+t_{B\,n+1}+(1-\gamma)t_{B\,n}\right]\right) \qquad \text{(IV-44)}$$

Thus, to calculate an average solution an average need only be computed once, and then used successively in equation IV-44, or the regular solution stepped out and averages calculated only for the points at the times where necessary.

The solution for an averaged method can be found by substituting in the defining equation IV-38 the solution as found from equation II-43 for the unaveraged method for times n and (n+1). For a problem which has a true steady-state solution we obtain

$$t_{n+k\ Ave} = t_P - C\ Q^n\left[\tfrac{1}{2}(Q+I)g\right] \qquad \text{(IV-45)}$$

where t_P, C, Q, and g are the identical quantities that are in the solution for the unaveraged method. By comparing equation IV-45 and equation II-43, the effect of averaging is to replace the initial vector g for the unaveraged method with the vector $\left[\tfrac{1}{2}(Q+I)g\right]$. If an eigenvalue q_j occurs that is close to (but greater than) -1 the component of $\left[\tfrac{1}{2}(Q+I)g\right]$ in the averaged method is significantly smaller in absolute value than that in g (see equation III-32). Consequently, the major advantage of averaging, regardless of the time at which the averaged solution is applied, is that the amplitude of the oscillations is significantly reduced. Therefore averaging is particularely useful for graphical methods the solution for which contains a negative q_{min} close to -1. Indeed, for some graphical methods applied to certain problems a q_{min} of -1 exists, and averaging is necessary to obtain a stable solution.

Although the form of the solution in equation IV-45 is useful to show the effect of averaging on the amplitude of the oscillations, to compare an averaged solution with the continuous solution a more convenient form is

$$t_{n+k\ Ave} = t_P - C\,Q^{n+k}\left[\tfrac{1}{2}Q^{-k}(I+Q)g\right] \qquad \text{(IV-46)}$$

which is used to examine positive damping factors only. The Q^{n+k} matrix corresponds directly to the $e^{-\nu^2(n+k)\Delta\tau}$ matrix in the continuous solution, and the effect of using the averaged temperature vector $t_{n+k\ Ave}$ at time $(n+k)\Delta\tau$ is to change the initial vector to $\left[\tfrac{1}{2}Q^{-k}(I+Q)g\right]$. The j^{th} component of this vector is $(q_j+1)g_j/2q_j^{\,k}$, which corresponds to a_j for the continuous solution and to g_j for the unaveraged approximate solution. For values of k of zero, or one, averaging changes components of the initial vector corresponding to q_j's of about 0.9 or larger from 2 to 5 per cent of the components in g_j; however, for the q_j's of about 0.6 to 0.7 the g_j's are significantly changed. When $k = \tfrac{1}{2}$ the components of the initial vector for the q_j larger than 0.9 are not significantly changed from those in the unaveraged vector g.

Interpolation. The interpolation technique was suggested by Longwell (20) for use with graphical methods to eliminate a certain type of oscillatory behavior. Some graphical methods including graphical method A, when applied to problems with a linear initial distribution and with either constant fluid temperature or adiabatic conditions, give a change in the temperature point only at alternate values of n. This gives a temperature-time graph that is a sequence of ramps and plateaus as in Figure IV-1(b). This condition is expressed, for example, by the equation for the temperature at a point as

$$t_{m,n-1} = t_{m,n} \neq t_{m,n+1} = t_{m,n+2} \qquad \text{(IV-47)}$$

For cases when this occurred it was suggested that the temperature at the end of a time increment during which no change occurred (at times n and (n+2) above) be replaced with a temperature linearly interpolated between those at the beginning of the previous time increment and the end of the next time increment. This gives for the above case at time n:

$$t_{m,n\,I} = \tfrac{1}{2}\left[t_{m,n-1} + t_{m,n+1}\right] \qquad \text{(IV-48)}$$

This then gives a sequence of ramps eliminating the plateaus.

Since $t_{m,n-1}$ and $t_{m,n}$ are equal the interpolated temperature is identical to a forward averaged temperature

$$t_{m,n\,I} = \tfrac{1}{2}\left[t_{m,n} + t_{m,n+1}\right] = t_{m,n\,Ave} \qquad k = 0 \qquad \text{(IV-49)}$$

Moreover, because $t_{m,n-1}$ and $t_{m,n}$ are equal and because interpolation does not change $t_{m,n-1}$, the forward average can be applied at the beginning of a plateau,

$$t_{m,n-1\,I} = t_{m,n-1} = \tfrac{1}{2}\left[t_{m,n-1} + t_{m,n}\right] = t_{m,n-1\,Ave} \qquad k = 0 \qquad \text{(IV-50)}$$

Consequently, if throughout the calculation each component of the temperature vector changes only at alternate time intervals, then using a forward average gives results equivalent to linear interpolation for those components which do not change.

Two points should be mentioned concerning the above discussion. First, although each component of the calculated temperature vector t_n changes only at alternate time increments, the vector t_n itself usually changes at each time increment. For example, in graphical method A applied to problem II, the odd-subscripted (m odd) components of t_n change only when n goes from odd to even and the even-subscripted (m even) components change only when n goes from even to odd; thus the vector t_n changes for each value of n, although some of its components remain constant for alternate values of n. The major conclusion is that the forward average is identical with interpolation for this case,

$$t_{n\,I} = \tfrac{1}{2}(t_n + t_{n+1}) = t_{n\,Ave} \qquad k = 0 \qquad \text{(IV-51)}$$

Secondly, a backward average applied to an approximate solution with a ramp-plateau temperature-time plot gives an approximation identical to using a linear interpolation for the temperature at the beginning of the plateau.

Modifications to Step Changes in Boundary Conditions. As noted in the Longwell paper (20), for problems with a constant initial temperature subjected to a constant different surface temperature, it has been suggested by many authors (6, 17) that a temperature half way between the initial temperature and the surface temperature can be used for the calculation from an n of zero to one. Then for all succeeding steps the actual surface temperature is used. For example, consider

a solid initially at zero temperature throughout, and at time zero. One surface temperature is held constant at unit temperature, the other boundary is insulated (problem II). The surface temperature for the continuous problem is:

$$T(0, n\Delta\tau) = 1 \qquad n \geq 0 \qquad \text{(IV-52)}$$

But instead of using in the difference calculation

$$t_{0,n} = 1 \qquad n \geq 0 \qquad \text{(IV-53)}$$

a ramp-step function defined by

$$t_{0,n} = \begin{cases} \frac{1}{2} & n = 0 \\ 1 & n \geq 1 \end{cases} \qquad \text{(IV-54)}$$

can be used to step out the solution. In the Longwell (20) work it was mentioned that this procedure for graphical method G gives the same results as interpolation for interpolated graphical method A for this problem. Hence we can conclude that for this case it is equivalent to an averaging technique.

This principle involved in modifying a constant boundary temperature can be generalized and applied to any problem where the fluid temperatures or the vector t_B are constant with time and where a boundary temperature vector $t_{B\ 0-}$ can be found that gives the initial temperature distribution as a steady-state solution. The last condition

can be expressed in difference form as either

$$Y\, t_0 = -Y_B\, t_{B\,0-} \tag{IV-55}$$

or

$$\left[I-\gamma\,\Delta\tau\,\frac{Y}{A}\right]t_0 = \left[I+(1-\gamma)\Delta\tau\,\frac{Y}{A}\right]t_0 + \Delta\tau\,\frac{Y_B}{A}\,t_{B\,0-} \tag{IV-56}$$

Since Y_B is a rectangular matrix the existence and uniqueness of $t_{B\,0-}$ is not guaranteed and depends upon the vector t_0. For a one-dimensional problem in Cartesian coordinates in a solid with uniform thermal properties $t_{B\,0-}$ exists only if the vector t_0 represents a linear distribution. Now the ramp-step procedure is to replace the vector $[(1-\gamma)t_{B\,n} + t_{B\,n+1}]$ that multiplies the matrix $\Delta\tau\, Y_B/A$ in equation II-39 with a ramp-step type function

$$(1-\gamma)t_{B\,n} + \gamma\, t_{B\,n+1} = \begin{cases} \frac{1}{2}(t_{B\,0-} + t_B) & n=0 \quad \text{(first step)} \\ t_B = \text{constant} & n \geq 1 \quad \text{(second and all other steps)} \end{cases} \tag{IV-57}$$

The equation for the first step becomes

$$t_{1,RS} = \left[I-\Delta\tau\,\frac{Y}{A}\right]^{-1}\left(\left[I+(1-\gamma)\Delta\tau\,\frac{Y}{A}\right]t_0 + \Delta\tau\,\frac{Y_B}{A}\left[\frac{t_{B\,0-} + t_B}{2}\right]\right) \tag{IV-58}$$

And using equation IV-55 to eliminate $t_{B\,0-}$ the equation is

$$t_{1,RS} = \left[I-\Delta\gamma\,\frac{Y}{A}\right]^{-1}\left(\left[I+(\tfrac{1}{2}-\gamma)\Delta\tau\,\frac{Y}{A}\right]t_0 + \Delta\tau\,\frac{Y_B}{A}\,\frac{t_B}{2}\right) \tag{IV-59}$$

This $t_{1,RS}$ is used to continue the stepping calculation. The averaged temperature vector $t_{0+k\ Ave}$ is found substituting t_1 from equation II-39 and t_0 into the definition giving:

$$t_{0+k\ Ave} = \tfrac{1}{2}\left\{\left[I-\gamma\Delta\tau\frac{Y}{A}\right]^{-1}\left(\left[I+(1-\gamma)\Delta\tau\frac{Y}{A}\right]t_0 + \Delta\tau\frac{Y_B}{A}t_B\right) + t_0\right\} \qquad \text{(IV-60)}$$

Combining the coefficients for t_0 and multiplying through by $\frac{1}{2}$ gives

$$t_{0+k\ Ave} = \left[I-\gamma\Delta\tau\frac{Y}{A}\right]^{-1}\left(\left[I+(\tfrac{1}{2}-\gamma)\Delta\tau\frac{Y}{A}\right]t_0 + \Delta\tau\frac{Y_B}{A}t_B\right) \qquad \text{(IV-61)}$$

which is the same expression as in equation IV-59 for $t_{1,rs}$; consequently,

$$t_{1,RS} = t_{0+k\ Ave} \qquad \text{(IV-62)}$$

Now, since using $t_{0+k\ Ave}$ to step out the rest of the solution gives an averaged solution according to equation IV-44, the same must be true when $t_{1,RS}$ is used. Further, if the averaged solution is assumed to apply at the end of the interval (k=1) then the backward average is identical to using the ramp-step modification for problems where the boundary temperature vector is constant and where the initial temperature distribution is a steady-state condition.

Conclusions and Averages to be Associated with Methods G, A, C, and F. The above discussion has shown that averaging the stepped-out solution for successive time increments greatly reduces the amplitude of the oscillations, but depending upon the time at which

the average is assumed to apply, the amplitude of the q_j's larger than 0.9 is not changed more than 5 per cent. Also, interpolation for approximate solutions with a ramp-plateau temperature-time plot and the replacement of a constant boundary vector with a ramp-step vector for problems with an initial condition, which fits a steady-state condition, are shown to be averaged methods. Since averaging can be applied to any problem or method it is a generalization of these two modifications.

Although the time at which an averaged solution applies is arbitrary, in order to be consistent with previous use of interpolation and the ramp-step modification, the backward average is used for methods G and C ; the forward average is used for methods A and F. Consequently, interpolation of graphical methods A and F is identical to averaging methods A and F for appropriate problems; and averaged methods G and C are identical to the ramp-step modification for appropriate problems. This also means that for problem II averaged methods A and G give identical results as do interpolated A and method G with a ramp-step modification as mentioned in reference (20).

(C) z-TRANSFORMS

The z-transform method of analysis of difference equations dates back to Heaviside and Laplace. Recently, it has been used in analyzing linear sampled-data control systems in electrical engineering and most of the properties derived here are shown in the texts of Aseltine (25), Jury (12), and Ragazzini and Franklin (13) on transform methods and sampled-data systems. In the following discussion the z-transforms are developed from the Laplace transforms and important properties are developed. This is not meant to be a rigorous mathematical discussion, but is meant to develop an understanding of the transforms. For purposes of reference, tables of z-transforms after Aseltine are reproduced (Tables IV-7 and IV-8).

A difference equation mathematically defines a function at only a point, and the function is not defined again until a certain increment of time or space has been traversed. (This obviously does not prevent us from interpolating between points.) For example, at a point m a temperature would only be defined at times $n\Delta\tau$, where n is an integer. This gives a sequence of impulses with zero width as shown in Figure IV-4.

The Laplace transform is defined by the equation (26)

$$\mathcal{L}\left\{f(\tau)\right\} = \int_0^\infty e^{-\tau s} f(\tau)d\tau \qquad \text{(IV-63)}$$

Considering that each impulse has an area associated with it equal to its magnitude, the Laplace transform integral of an impulse is, under these assumptions,

$$\int_{n\Delta\tau-}^{n\Delta\tau+} e^{-s\tau} f_n \, d\tau = (e^{-s\Delta\tau})^n f_n \tag{IV-64}$$

Therefore the Laplace transform of the sequence of impulses or of a difference signal is:

$$\mathcal{L}\left\{f_n\right\} = \int_0^{\infty} e^{-s\tau} f_n \, d\tau = \sum_{n=0}^{\infty} f_n e^{-sn\Delta\tau} \tag{IV-65}$$

Now, making the substitution

$$z = e^{s\Delta\tau} \tag{IV-66}$$

the expression becomes

$$\mathcal{L}\left\{f(n\Delta\tau)\right\} = \sum_{n=0}^{\infty} z^{-n} f(n\Delta\tau) = \sum_{n=0}^{\infty} f_n z^{-n} \tag{IV-67}$$

$$= f_0 + f_1 z^{-1} + f_2 z^{-2} + \ldots + f_n z^{-n} + \ldots$$

The z-transform is defined as the Laplace transform of a sampled signal, having an area equal to its magnitude, with the substitution z for $e^{s\Delta\tau}$ as given by equation IV-66. This definition is then

$$\mathcal{Z}\left\{f_n\right\} = \bar{f}(z) = \sum_{n=0}^{\infty} f_n z^{-n} \tag{IV-68}$$

The z-transform may be defined directly by the above relationship independently of the Laplace transform. As with the Laplace transform the difference signal is assumed to be zero for all n less than zero. The relationship between the Laplace transform and the z-transform is useful and the relationship in equation IV-66 is actually a mapping from the complex s-plane to the complex z-plane. For example, the imaginary axis of the s-plane is repeatedly mapped onto the unit circle in the z-plane; thus poles located in the area left of this axis in the s-plane for a stable solution are mapped inside the unit circle of the z-plane, which is the requirement of stability for the difference system. Also the z-transform of a signal sampled from a continuous signal may be found by a complex integration of the Laplace transform of the continuous signal times the transform of sequences of pulses (12, 13).

To show how the z-transform may be manipulated, a few of the important transform pairs will be briefly developed. For a unit step function that is zero for n less than zero, but one for all n equal to or greater than zero we would have

$$f_n = \begin{cases} 0 & n < 0 \\ 1 & n \geq 0 \end{cases} \qquad \text{(IV-69)}$$

$$\bar{f} = \mathcal{Z}\{f_n\} = \sum_{n=0}^{\infty} z^{-n} = 1 + z^{-1} + z^{-2} + \ldots + z^{-n}$$

$$= \frac{z}{z-1} \qquad \text{(IV-70)}$$

The last equality comes from Dwight (27), equation 9.04.

One of the most important Laplace transform relationships is that for a simple pole

$$\mathcal{L}\left\{ e^{\lambda \tau} \right\} = \frac{1}{s - \lambda} \tag{IV-71}$$

which includes the trigonometric interpretations if λ is considered to be complex. The corresponding z-transform is

$$\mathcal{Z}\left\{q^n\right\} = \sum_{n=0}^{\infty} q^n z^{-n} = 1 + q z^{-1} + q^2 z^{-2} + \ldots + q^n z^{-n} = \frac{z}{z - q} \tag{IV-72}$$

Again, if q is considered a complex number the above transform has corresponding interpretations in cosine and sine functions. Simple transforms are inverted using equation IV-72 and partial fractions. The third important relationship is the shifting property, which can be found starting from:

$$\mathcal{Z}\left\{f_{n+1}\right\} = \sum_{n=0}^{\infty} f_{n+1} z^{-n} = z \sum_{n=0}^{\infty} f_{n+1} z^{-(n+1)} \tag{IV-73}$$

Now change variable of summation by

$$p = n + 1 \tag{IV-74}$$

Then,

$$\mathcal{Z}\left\{f_{n+1}\right\} = z \sum_{p=1}^{\infty} f_p z^{-p} \tag{IV-75}$$

And adding and subtracting $(z\, f_0)$ on the right side of the equation:

$$\mathcal{Z}\left\{f_{n+1}\right\} = -z\, f_0 + z \sum_{p=0}^{\infty} f_p\, z^{-p} \qquad \text{(IV-76)}$$

which gives the shifting property:

$$\mathcal{Z}\left\{f_{n+1}\right\} = z\, \bar{f}_n - z\, f_0 \qquad \text{(IV-77)}$$

This relationship shows that the multiplying by z is analogous to multiplying by the advancing difference operator* E, as multiplying by s is analogous to multiplying by the operator $d/d\tau$.

To invert transforms not in the table an inversion theorem is used. This theorem is based on a Cauchey formula (12) for contour integration in the complex plane which is:

$$\frac{1}{2\pi\sqrt{-1}} \int_{\Gamma} z^p\, dz = \begin{cases} 0 & p > -1 \\ 1 & p = -1 \\ 0 & p < -1 \end{cases} \qquad \text{(IV-78)}$$

where Γ is a closed curve enclosing the origin. To use this integral first we multiply the definition of the z-transform by z^{n-1} obtaining

$$z^{n-1}\, \bar{f}(z) = f_0 z^{n-1} + f_1 z^{n-2} + \ldots + f_{n-1} z^0 + f_n z^{-1} + f_{n+1} z^{-2} + \ldots \qquad \text{(IV-79)}$$

Now integrating both sides of equation IV-79 along a closed contour in the z-plane we obtain

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* E defined by: $E\, f_n = f_{n+1}$

$$f_n = \frac{1}{2\pi\sqrt{-1}} \int_{\Gamma} z^{n-1} \bar{f}(z)dz \qquad \text{(IV-80)}$$

The closed curve, Γ, must enclose all singularities of $z^{n-1} \bar{f}(z)$.

The usual circumstance is that all the singularities are poles and the integration path is taken as a circle enclosing them; this contour for a stable solution is the unit circle and is shown in Figure IV-5(a). In this case, the integral in equation IV-80 is evaluated directly from the residue theorem and the inversion is

$$f_n = \sum_{j=0}^{\infty} \text{residues of poles of } z^{n-1} \bar{f}(z) = \sum_{j=0}^{\infty} \rho_{j,n} \qquad \text{(IV-81)}$$

where $\rho_{j,n}$ = residues of $z^{n-1} \bar{f}(z)$ and the summation is over all the poles of $z^{n-1} \bar{f}(z)$.

The residue for simple poles (28) is

$$\rho_{j,n} = \lim_{z \to q_j} (z-q_j) z^{n-1} \bar{f}(z) \qquad \text{(IV-82)}$$

or

$$\rho_{j,n} = \lim_{z \to q_j} \frac{N(z)}{dD(z)/dz} \qquad \text{(IV-83)}$$

where

$$z^{n-1} \bar{f}(z) = \frac{N(z)}{D(z)}$$

$N(z)$ = numerator of $z^{n-1} \bar{f}(z)$; may contain elements of denominator as long as it is analytic as $z \to q_j$

$D(z)$ = denominator of $z^{n-1}\bar{f}(z)$ not contained in $N(z)$; goes to zero as $z \to q_j$

For a pole with multiplicity of μ the residue (28) is:

$$\rho_{j,n} = \lim_{z \to q_j} \left[\frac{1}{(\mu-1)!} \frac{\partial^{\mu-1}}{\partial z^{\mu-1}} \left\{ z^{n-1}(z-q_j)^{\mu} \bar{f}(z) \right\} \right] \qquad \text{(IV-84)}$$

Another form of equation IV-84 is found by using the formula for higher-order derivatives of a product.

$$\rho_{j,n} = \lim_{z \to q_j} \sum_{p=1}^{\mu} \frac{(n-1)! \; (z^{n-p}) \frac{d^{\mu-p}}{dz^{\mu-p}} \left\{ (z-q_j)^{\mu} \bar{f}(z) \right\}}{(n-p)! \; (\mu-p)! \; (p-1)!} \qquad \text{(IV-85)}$$

For the case of a pole with multiplicity of 2 an equation of the form of equation IV-83 is useful (28):

$$\rho_{j,n} = 2 \lim_{z \to q_j} \left[\frac{\frac{dN(z)}{dz}}{\frac{d^2 D(z)}{dz^2}} - \frac{N(z) \; \frac{d^3 D(z)}{dz^3}}{3 \left(\frac{d^2 D(z)}{dz^2} \right)^2} \right] \qquad \text{(IV-86)}$$

In some cases, the use of the above equations to invert $\bar{f}(z)$, summing only the residues of the singularities of $\bar{f}(z)$, gives a solution that agrees with the stepped-out calculations only for n's greater than some low number, n_1, where n_1 is usually zero. That is, the resulting solution fails to fit the assumed initial condition and the stepped-out

calculations up through increment n_1. The reason for this is that the inversion integration must be done on $z^{n-1}\bar{f}(z)$, not $\bar{f}(z)$, and that $z^{n-1}\bar{f}(z)$ may have a singularity at zero, or may have a higher-order singularity at zero than does $\bar{f}(z)$. But, since in this study of the partial difference equation of diffusion, we are not usually interested in the solution for $n = 0$ or 1, but only for the intermediate and large values of n, the residue of this singularity can be neglected. However, so that this apparent inconsistency does not cast doubt on the z-transform technique, the following two paragraphs show first, when this singularity occurs, and second, how to find the additional terms which when added to the residues of $\bar{f}(z)$ give the solution that is correct for all values of n.

Assuming that $\bar{f}(z)$ can be written as a ratio of polynomials in z, as is the usual case, then the behavior of $\bar{f}(z)$ as z goes to zero determines the existence and order of this singularity of $z^{n-1}\bar{f}(z)$. If $\bar{f}(z)$ goes to zero as z goes to zero, $z^{n-1}\bar{f}(z)$ must be analytic for all $n = 0, 1, \ldots, \infty$ at a z of zero. However, if $\bar{f}(z)$ goes to neither zero nor infinity as z goes to zero, $z^{n-1}\bar{f}(z)$ contains a simple pole at zero when n is zero. Here the sum of the residues of $\bar{f}(z)$ gives a solution valid for $n > 0$. If $\bar{f}(z)$ itself contains a pole at $z = 0$ of multiplicity n_1, $z^{n-1}\bar{f}(z)$ has a pole at $z = 0$ with multiplicity $(n_1 + 1)$ for an n of zero, and the sum of the residues of $\bar{f}(z)$ gives a solution valid for $n > n_1$.

In order to find the inversion relationship of a multiple pole at zero, the definition of the z-transform and the Kronecker delta function can be combined to give

$$\mathcal{Z}\left\{\delta_{n,p}\right\} = z^{-p} \qquad n = 0, 1, \ldots, \infty \qquad \text{(IV-87)}$$

where $\delta_{n,p} \equiv 0 \quad n \neq p$

$\qquad\qquad\quad 1 \quad n = p$

p = non-negative constant integer

Note that a constant term in the transform would give an impulse at an n of zero, $\delta_{n,0}$, because of the singularity introduced by z^{n-1}. If the transform can be written in terms of partial fractions the inversion is simply accomplished using this relationship and equations IV-87 and IV-72. For the complicated transforms that result from the diffusion problem this cannot be done conveniently. In these cases equation IV-82 may be used to find the residue of the zero pole. Since we are applying this to $z^{n-1}\bar{f}(z)$ the multiplicity of the zero pole is $(n_1 + 1)$ where n_1 is the multiplicity of zero pole for $\bar{f}(z)$; (n_1 must be zero or positive; if it is negative there is no singularity at zero). As an example, using equation IV-84 to invert the transform z^{-1} with a simple pole ($\mu = 2$), we obtain

$$\lim_{z \to 0} \frac{1}{1!} \frac{\partial}{\partial z}\left\{z^{n-1} z^{2} z^{-1}\right\} = \lim_{z \to 0} \frac{\partial}{\partial z} z^{n} = \lim_{z \to 0} n(z)^{n-1} = n(0)^{n-1} \qquad \text{(IV-88)}$$

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

Although the term $n(0)^{n-1}$ is indeterminate for an n of zero, it is actually a short way of representing the limit of $n(z)^{n-1}$ as z goes to zero. Taking that limit using l'Hospital's rule for n of zero and usual definitions for other values of n this result is equivalent to equation IV-87

$$\delta_{n,1} = n(0)^{n-1} \qquad n = 0, 1, \ldots, \infty \qquad \text{(IV-89)}$$

As analogous arguments are valid for a higher-order pole at zero, it is concluded that this approach is valid and equivalent to using partial fractions to invert the transform for determining this residue.

A second type of singularity that can occur is a branch cut. The inversion of a transform of this type is like the procedure used when a branch cut occurs with Laplace transforms. The inversion integration is carried out on a closed curve that excludes the branch point and other singularities, but part of the path is a circle that would in a limit enclose the origin. ABCDA in Figure IV-5(b) is such a path for a branch cut from -1 to +1. The details of such an integration are shown in section D-4 of this chapter by an example.

A simple numerical method for the transform inversion is to generate the definition series equation IV-68. The coefficient of each $z^{-0}, z^{-1}, \ldots, z^{-n}$ is then $f_0, f_1, \ldots, f_n$. This may be simply done by arranging the transform as a ratio of polynomials in z^{-1} and carrying

out the long division. This procedure is often useful in checking the algebra used to derive the transform. Also by a simple examination of the definition the initial value theorem is derived,

$$\lim_{n \to 0} f_n = \lim_{z \to \infty} \bar{f}(z) \qquad \text{(IV-90)}$$

This theorem is used in checking derived transforms.

This brief discussion on the z-transform is not a presentation of rigorous proofs but is intended to show the development of z-transforms from the Laplace transforms, the important transform pairs, and the inversion. For a more rigorous treatment, any of the three texts mentioned should be consulted, particularly for such questions as uniqueness and restrictions on the types of functions. Texts (28) on complex variables are also useful.

(D) z-TRANSFORMS AND PARTIAL DIFFERENCE EQUATIONS--EXAMPLE PROBLEMS

The z-transform procedure for solving a partial difference equation is identical to that required for the Laplace transform procedure of solving a partial differential equation. The procedure is:

(1) Transform the partial difference equation with respect to the independent variable for which the initial values are known. This gives a difference equation with one less independent variable.

(2) Transform any boundary condition equations together with their initial conditions.

(3) Solve the transformed difference equation with the boundary conditions to obtain an explicit form for the transformed dependent variable.

(4) Invert the transform by using the tables or the inversion theorem to find the analytic solution of the partial difference equation. As z-transforms are not well known, the tables available are not as complete as those for the Laplace transform and usually the inversion theorem is required, particularly for the transforms obtained from the partial difference equation for diffusion.

Since the z-transform method of solving partial difference equations has not been found published, several related difference problems are now solved in detail to demonstrate the technique and the manipulations required. The problems selected are not the simplest possible,

but they show many of the difficulties encountered, how to overcome them, and where simplifications are possible. Most steps are carried out in some detail with discussion of special problems in addition to simplifications. In the earlier part of the problem the equations are kept in the most general form for as long as possible.

1. Problem I--Finite H, Method G

The difference problem to be solved involves a one-dimensional solid. Method G, Table IV-1, will be used to approximate a continuous problem with an arbitrary initial condition. The left boundary (x=0) is in contact with a fluid with a finite heat-transfer coefficient and whose temperature is specified as a function of time. The right boundary (x=L) is adiabatic. Method G uses mesh $\Delta\xi$ in Figure IV-2 with points located at both boundaries and uniformly spaced and it is defined in detail in Table IV-1. The arbitrary initial condition for the difference method is represented by $t_{m,0}$, where m goes from 0 to S corresponding to ξ from 0 to 1, and the fluid temperature is represented by $t_{f,n}$. Since to obtain a solution using z-transforms it is necessary to specify the initial distribution and how the fluid temperature changes with time, these conditions are taken as:

$$t_{m,0} = 0 \qquad 0 \leq m \leq S \tag{IV-91}$$

$$t_{f,n} = 1 \qquad n \geq 0 \tag{IV-92}$$

This is problem I as described in Table IV-9. However, these specific conditions are not introduced into the equations until necessary. After solving the specific problem above, the following related problems are shown based on method G. First, the solution is modified to an averaged method G. Second, the case for specified boundary condition or infinite heat-transfer coefficient is shown. Then the solution for an explicit method for a semi-infinite solid is shown.

The one-dimensional partial difference equation for diffusion in general form, equation II-42, is:

$$-r\gamma t_{m-1,n+1} + (1+2r\gamma)t_{m,n+1} - r\gamma t_{m+1,n+1} = r(1-\gamma)t_{m-1,n} + [1-2r(1-\gamma)]t_{m,n} + r(1-\gamma)t_{m+1,n} \qquad \text{(IV-93)}$$

$$m = 1, 2, \ldots, S-1$$

$$n = 0, 1, 2, \ldots, \infty$$

The boundary equations for the finite h at point zero and zero h at point S for method G are, respectively:

$$\left[1+2r\gamma\left(1+\frac{H}{S}\right)\right]t_{0,n+1} - 2r\gamma t_{1,n+1} = \left[1-2r(1-\gamma)\left(1+\frac{H}{S}\right)\right]t_{0,n} + 2r(1-\gamma)t_{1,n} + 2r\frac{H}{S}\left[(1-\gamma)t_{f,n} + \gamma t_{f,n+1}\right]$$

$$n = 0, 1, \ldots, \infty \qquad \text{(IV-94)}$$

$$(1+2r\gamma)t_{S,n+1} - 2r\gamma t_{S-1,n+1} = [1-2r(1-\gamma)]t_{S,n} + 2r(1-\gamma)t_{S-1} \qquad \text{(IV-95)}$$

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

where $H = hL/k$.

A significant simplification in the adiabatic boundary equation IV-95 can be made by writing the partial difference equation IV-93 for point S, which requires the introduction of an imaginary point at (S+1). Subtracting the boundary equation IV-95 from the partial difference equation the result is simply:

$$r\gamma(t_{S-1,n+1} - t_{S+1,n+1}) = r(1-\gamma)(-t_{S-1,n} + t_{S+1,n}) \qquad \text{(IV-96)}$$

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

Since the imaginary point (S+1) must have the same initial condition as point (S-1) we have simply

$$t_{S+1,n} = t_{S-1,n} \qquad n = 0, 1, \ldots, \infty \qquad \text{(IV-97)}$$

With this modification, the partial difference equation IV-93 is written for point S. The method for simplifying the adiabatic boundary condition could be used to modify the other heat-transfer coefficient condition, but as long as the coefficient is not zero no simplification is obtained.

Now that the partial difference equation and the boundary conditions have been simplified, they can be transformed using the relationships in the table. The transformed equations are, with no

simplification, in terms of the arbitrary initial condition and fluid temperature for equations IV-93, IV-94, and IV-97, respectively:

$$-r\gamma z[\bar{t}_{m-1} - t_{m-1,0} + \bar{t}_{m+1} - t_{m+1,0}] + (1+2r\gamma)z[\bar{t}_m - t_{m,0}] =$$

$$r(1-\gamma)[\bar{t}_{m-1} + \bar{t}_{m+1}] + [1-2r(1-\gamma)]\bar{t}_m \qquad \text{(IV-98)}$$

$$m = 1, 2, \ldots, S-1, S$$

$$z\left[1+2r\gamma\left(1+\frac{H}{S}\right)\right][\bar{t}_0 - t_{0,0}] - 2r\gamma z[\bar{t}_1 - t_{1,0}] =$$

$$\left[1-2r(1-\gamma)\left(1+\frac{H}{S}\right)\right]\bar{t}_0 + 2r(1-\gamma)\bar{t}_1 \qquad \text{(IV-99)}$$

$$+ 2r\frac{H}{S}\left[(1-\gamma)\bar{t}_f + \gamma z(\bar{t}_f - t_{f,0})\right]$$

$$\bar{t}_{S+1} = \bar{t}_{S-1} \qquad \text{(IV-100)}$$

A more convenient form for equations IV-98 and IV-99 is found by rearranging and combining terms so that the unknown transformed variables are on the left side and the known quantities and functions specified by the initial and boundary conditions are on the right.

$$\bar{t}_{m-1} - \left[\frac{z-1+2r(z\gamma+1-\gamma)}{r(z\gamma+1-\gamma)}\right]\bar{t}_m + \bar{t}_{m+1} =$$

$$\frac{z}{r(z\gamma+1-\gamma)}\left[r\gamma(t_{m-1,0} + t_{m+1,0}) - (1+2r\gamma)t_{m,0}\right] \qquad \text{(IV-101)}$$

$$m = 1, 2, \ldots, S-1, S$$

$$\left[z+1+2r\left(1+\frac{H}{S}\right)(\gamma z+1-\gamma)\right]\bar{t}_0 - 2r(\gamma z+1-\gamma)\bar{t}_1 =$$

$$\frac{2rH}{S}(\gamma z+1-\gamma)\bar{t}_f \qquad \text{(IV-102)}$$

$$+ z\left[\left\{1+2r\gamma\left(1+\frac{H}{S}\right)\right\}t_{0,0} - 2r\gamma t_{1,0} - 2r\frac{H\gamma z}{S}t_{f,0}\right]$$

$$\bar{t}_{S+1} = \bar{t}_{S-1} \qquad \text{(IV-103)}$$

These three equations are, respectively, a second-order ordinary difference equation, IV-101, and its two boundary condition equations, IV-102 and IV-103. The first equation is the transformed one-dimensional diffusion difference equation for any initial distribution.

Application of Initial Conditions. In order to find the solution of the difference equation IV-101 and its boundary equations IV-102 and IV-103, the initial conditions $t_{m-1,0}$, $t_{m+1,0}$, and $t_{m,0}$ must be expressed as functions of m and in a form that applies for each value of m for which the difference equation applies. In equation IV-101 if γ is not zero an expression for $t_{m,0}$ must apply for m of 0 to (S+1) even though the difference equation applies for m from 0 to S. In most cases, a suitable function of m may be obtained directly from the initial distribution for the continuous problem. However, in some cases, particularly when the surface temperature is specified, the required expression is not obvious. Consider for a moment the case when the surface temperature $t_{0,0}$ is specified as one, but the initial

temperature distribution $t_{m,0}$ for $m = 1, \ldots (S+1)$ is zero. In this case a suitable function that fits the initial distribution is:

$$t_{m,0} = \delta_{m,0} \qquad m = 0, 1, \ldots, S \qquad \text{(IV-104)}$$

where $\delta_{m,p}$ = Kronecker delta function = $\begin{cases} 1 & m = p \\ 0 & m \neq p \end{cases}$

(Note second subscript on δ does not refer to time in this case as does the second subscript on t.) In general, a series of terms using the Kronecker delta function may be used:

$$t_{m,0} = \sum_{p=0}^{S} t_{p,0}\, \delta_{m,p} \qquad m = 0, 1, \ldots, S \qquad \text{(IV-105)}$$

If an analytic expression for the Kronecker delta function is necessary to allow a solution of the difference equation, either a form with 0 roots or the Lagrangian interpolation formula may be satisfactory, but both are complicated. These are, respectively,

$$\delta_{m,p} = \frac{m(m-1) \ldots (m-p+1)(0)^{m-p}}{p!} \qquad m,p = 0, 1, \ldots, S \qquad \text{(IV-106)}$$

$$\delta_{m,p} = \frac{m(m-1) \ldots (m-p+1)(m-p-1) \ldots (m-S)}{p(p-1) \ldots (1)(-1) \ldots (p-S)} \qquad m,p = 0, 1, \ldots, S \qquad \text{(IV-107)}$$

In equation IV-106 to keep the term $[m(m-1) \ldots (m-p+1)(0)^{m-p}]$ finite for m less than p, it is considered as the limit of

$[m(m-1) \ldots (m-p+1)\,(\epsilon)^{m-p}]$ as ϵ goes to zero as used in equation IV-89. For mesh $\Delta\xi/2$ the variable m would be replaced by $(m - \frac{1}{2})$.

Another method that avoids the series above is to first solve the explicit case ($\gamma = 0$). The partial difference equation is then

$$\bar{t}_{m-1} - \left(\frac{z-1+2r}{r}\right)\bar{t}_m + \bar{t}_{m+1} = \frac{-z}{r}\, t_{m,0} \qquad m = 1, 2, \ldots, S \quad \text{(IV-108)}$$

In this case, the expression for the initial distribution does not need to fit the initial boundary temperature $t_{0,0}$ as the equation applies only to $m = 1, 2, \ldots, S$. The boundary equation allows for the initial boundary temperature in equation IV-102 for point 1, which can be rewritten for zero γ:

$$\left[z-1+2r\left(1+\frac{H}{S}\right)\right]\bar{t}_0 - 2r\bar{t}_1 = \frac{2rH}{S}\,\bar{t}_f + z t_{0,0} \qquad \text{(IV-109)}$$

The solution for the explicit case is found; then, by setting n to zero in this solution an expression results which fits the initial condition for all $m = 0, 1, \ldots, (S+1)$: This expression is then substituted in equations IV-101 and IV-102 for the implicit case. Although this expression is a series, because of the way it was found, it simplifies the solution of the original system of equations IV-101, IV-102, and IV-103.

For cases where the Y/A matrix and the particular solution are not functions of the time differencing parameters $\Delta\tau$ and γ, an additional simplification can often be made. Here, in addition to the particular solution, neither the eigenvectors of the Y/A matrix nor the initial vectors are functions of the time differencing parameters. Consequently,

these quantities can be found by using the z-transform to solve the problem for a convenient combination of time increment $\Delta\tau$ and weighting γ; this usually corresponds to an r of $\frac{1}{2}$ and a γ of zero. This solution also gives the q_j's that correspond to the specific time differencing parameters used, and the eigenvalues of the Y/A matrix, λ_j, are then found from equation II-56. Once these values are known, the Q matrix for any combination of $\Delta\tau$ and γ is known from equation II-57 and the analog solution is obtained by replacing the Q^n matrix with the $e^{+\Lambda\tau}$ matrix. This latter fact means that in these cases the Laplace transform could be applied to the analog system of differential equations.

$$\frac{d\,t_m}{d\tau} = \frac{1}{(\Delta\xi)^2}\left[t_{m-1} - 2t_m + t_{m+1}\right] \qquad \text{(IV-110)}$$

together with the analog boundary conditions. After taking the Laplace transform this gives a boundary value ordinary difference problem as found in equations IV-101, IV-102, and IV-103. Solving these equations and inverting the Laplace transform gives the eigenvectors and initial vector for the approximate method and the eigenvalues λ_j from which not only the analog solution is found, but also the Q matrix for the difference solution can be found. These simplifications can be applied to methods G and C as applied to problems where a true steady-state solution exists.

Solution of Transformed Difference Equation. Returning to the example problem, to solve the ordinary difference equation we take the initial temperature distribution as zero at all points,

$$t_{m,0} = 0 \qquad 0 \le m \le S+1 \tag{IV-111}$$

Thus the equations IV-101, IV-102, and IV-103 become,

$$\bar{t}_{m-1} - \left[\frac{z-1+2r(z\gamma+1-\gamma)}{r(z+1-\gamma)}\right]\bar{t}_m + \bar{t}_{m+1} = 0 \tag{IV-112}$$

$$m = 1, 2, \ldots, S, S+1$$

$$\left[z-1+2r\left(\frac{H}{S}+1\right)(\gamma z+1-\gamma)\right]\bar{t}_0 - 2r(\gamma z+1-\gamma)\bar{t}_1 = 2r\frac{H}{S}\left[(\gamma z+1-\gamma)\bar{t}_f - z\gamma t_{f,0}\right] \tag{IV-113}$$

$$\bar{t}_{S-1} = \bar{t}_{S+1} \tag{IV-114}$$

The difference equations IV-101, IV-102, and IV-103 are more easily solved with the following definition (15, 21):

$$\cos\alpha = \frac{z-1+2r(z\gamma+1-\gamma)}{2r(z\gamma+1-\gamma)} \tag{IV-115}$$

or inversely

$$z = \frac{1-2r(1-\gamma)(1-\cos\alpha)}{1+2r\gamma(1-\cos\alpha)} \tag{IV-116}$$

Substitution gives, simply, for the difference equation IV-112

$$\bar{t}_{m+1} - 2\cos\alpha\,\bar{t}_m + \bar{t}_{m-1} = 0 \qquad m = 1, 2, \ldots, S, S+1 \tag{IV-117}$$

The transformed boundary equation is simplified by solving equation IV-116 for (z-1)

$$z-1 = 2r(\gamma z+1-\gamma)(1-\cos\alpha) = \frac{2r(\cos\alpha-1)}{1+2r\gamma(1-\cos\alpha)} \qquad \text{(IV-118)}$$

Substituting this in the coefficient for $\bar{t}_0$ in equation IV-113 gives:

$$\left\{\cos\alpha+\frac{H}{S}\right\}\bar{t}_0 - \bar{t}_1 = \frac{H}{S(\gamma z+1-\gamma)}\left[(\gamma z+1-\gamma)\,\bar{t}_f - z\gamma t_{f,0}\right] \qquad \text{(IV-119)}$$

The solution of the homogeneous equation IV-117 is:

$$\bar{t}_m = P\cos m\alpha + G\sin m\alpha \qquad m = 0,\ 1,\ \ldots,\ S,\ S+1 \qquad \text{(IV-120)}$$

where P and G are constants to be found from the two boundary relationships or their modified forms, equations IV-114 and IV-119, so that the solution also satisfies these boundary equations. If a non-zero initial condition were present, equation IV-117 would not be homogeneous and a particular solution found by the method of undetermined parameters would be added to the above complementary solution.

To evaluate the constants P and G we first find the expressions for $\bar{t}_{S+1}$ and $\bar{t}_{S-1}$ from equation IV-120 by setting m equal to (S+1) and (S-1), respectively.

$$\bar{t}_{S+1} = P\cos(S+1)\alpha + G\sin(S+1)\alpha \qquad \text{(IV-121)}$$

$$\bar{t}_{S-1} = P\cos(S-1)\alpha + G\sin(S-1)\alpha \qquad \text{(IV-122)}$$

and substituting them in the boundary equation IV-114 gives:

$$\bar{t}_{S+1} - \bar{t}_{S-1} = 0 = P\cos(S+1)\alpha + G\sin(S+1)\alpha - P\cos(S-1)\alpha - G\sin(S-1)\alpha \quad \text{(IV-123)}$$

Simplifying with trigonometric identities gives

$$P\tan S\alpha = G \quad \text{(IV-124)}$$

Now G is eliminated from equation IV-120 which, using trigonometric identities, gives

$$\bar{t}_m = \frac{P\cos(S-m)\alpha}{\cos S\alpha} \quad \text{(IV-125)}$$

From equation IV-125 the transforms $\bar{t}_0$ and $\bar{t}_1$ are:

$$\bar{t}_0 = \frac{P\cos S\alpha}{\cos S\alpha} \quad \text{(IV-126)}$$

$$\bar{t}_1 = \frac{P\cos(S-1)\alpha}{\cos S\alpha} \quad \text{(IV-127)}$$

and substituting them in equation IV-119 gives:

$$\frac{P}{\cos S\alpha}\left[\left(\cos\alpha + \frac{H}{S}\right)\cos S\alpha - \cos(S-1)\alpha\right] = \frac{H}{S(\gamma z+1-\gamma)}\left[(\gamma z+1-\gamma)\bar{t}_f - z\gamma\bar{t}_{f,0}\right] \quad \text{(IV-128)}$$

Solving for $P/\cos S\alpha$ and substituting in equation IV-125 together with trigonometric simplification of the bracketed form on the left gives the solution for the transformed difference temperature.

$$\bar{t}_m = \frac{H}{S}\left[\frac{(\gamma z+1-\gamma)\bar{t}_f - z\gamma t_{f,0}}{\gamma z+1-\gamma}\right]\left[\frac{\cos(S-m)\alpha}{\frac{H}{S}\cos S\alpha - \sin S\alpha \sin\alpha}\right] \qquad \text{(IV-129)}$$

At this point, it is usually advantageous to check the solution in the boundary equations, and also to check the initial conditions using the initial value theorem, item 14, Table IV-7.

Inversion of Transform. The next and last step is the inversion of the transform. To do this we specify how the fluid temperature varies with time. Assuming that it is constant at unity for all n equal to and greater than zero we have from item 1, Table IV-8:

$$\bar{t}_f = \frac{z}{z-1} \qquad \text{(IV-130)}$$

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

$$t_{f,n} = 1$$

Substituting in the transform temperature in equation IV-129,

$$\bar{t}_m = \left[\frac{z}{(z-1)(\gamma z+1-\gamma)}\right]\left[\frac{H\cos(S-m)\alpha}{H\cos S\alpha - S\sin S\alpha \sin\alpha}\right] \qquad \text{(IV-131)}$$

The inversion theorem must be used to find $t_{m,n}$. The quantity $(z^{n-1}\bar{t}_m)$ has only poles for singularities. These poles occur at values of z for which the quantities (z-1) and $(H\cos S\alpha - S\sin\alpha \sin S\alpha)$ go to zero. Although it appears that $(z\gamma+1-\gamma)$ gives another pole, we will show first that $\bar{t}_m$ is actually analytic at a z of $(\gamma-1)/\gamma$; then we will discuss the roots of the trigonometric quantity and evaluate the residues.

To show that $(\gamma-1)/\gamma$ is not a pole of $\bar{t}_m$, from trigonometric identities and the definition of $\cos\alpha$:

$$\sin\alpha = \frac{\sqrt{-(z-1)(z-1+4r\{\gamma z+1-\gamma\})}}{2r(z\gamma+1-\gamma)} \qquad \text{(IV-132)}$$

Now from the formulas for sine and cosine of multiple angles we know that $\cos(S-m)\alpha$ is a polynomial that contains $(\cos\alpha)$ to the $(S-m)$ power; $(\cos S\alpha)$ contains $(\cos\alpha)$ to the S power; $(\sin S\alpha)$ contains $(\sin\alpha)$ to the S power or $(\cos\alpha)$ times $(\sin\alpha)$ to the $(S-1)$ power, depending on S odd or even. Thus, since both $(\cos\alpha)$ and $(\sin\alpha)$ contain the factor $(\gamma z+1-\gamma)$ in the denominator, the term $(H\cos S\alpha - S\sin\alpha\sin S\alpha)$ is a polynomial that contains the factor $(\gamma z+1-\gamma)$ to the $(S+1)$ power in its denominator; and $\cos(S-m)\alpha$ with $(\gamma z+1-\gamma)$ to the $(S-m)$ power in its denominator. Consequently, $\bar{t}_m$ would contain $(\gamma z+1-\gamma)$ to the $[S+1-(S-m)-1]$ or to the m^{th} power in its numerator; and as z goes to $(\gamma-1)/\gamma$, $\bar{t}_m$ has a limit; therefore, $\bar{t}_m$ is analytic for all m from 0 to $(S+1)$.

Next the residue at a z of one is evaluated using equation IV-82. Note that in taking limits as z goes to one we must also evaluate α which, from equation IV-115, goes to 0.

$$\lim_{z\to 1}\cos\alpha = \lim_{z\to 1}\left[\frac{z-1+2r(\gamma z+1-\gamma)}{2r(\gamma z+1-\gamma)}\right] = 1 = \cos(0) \qquad \text{(IV-133)}$$

$$\rho_{1,n} = \lim_{\substack{z\to 1\\ \alpha\to 0}} (z-1)z^{n-1}\,\bar{t}_m = \lim_{\substack{z\to 1\\ \alpha\to 0}} \left\{ \frac{z^n H\cos(S-m)\alpha}{(\gamma z+1-\gamma)(H\cos S\alpha - S\sin\alpha\sin S\alpha} \right\} \qquad \text{(IV-134)}$$

$$= 1$$

This corresponds to the steady-state or particular solution.

The roots of the quantity ($H\cos S\alpha - S\sin\alpha\sin S\alpha$) are the poles for the transient part of the solution and must satisfy

$$S\sin\alpha_j \tan S\alpha_j = H \qquad j = 1, 2, \ldots, S+1 \qquad \text{(IV-135)}$$

Using the relationship between z and α, equation IV-116 gives:

$$\lim_{\substack{\alpha\to\alpha_j\\ z\to q_j}} z = q_j = \frac{1-2r(1-\gamma)(1-\cos\alpha_j)}{1+2r\gamma(1-\cos\alpha_j)} \qquad \text{(IV-136)}$$

$$j = 1, 2, \ldots, S+1$$

We can write the $j = 1, 2, \ldots, (S+1)$, because method G has a Y/A matrix of dimension (S+1) by (S+1) and we know from equation IV-135 that (S+1) eigenvalues or q_j's exist. Assuming that the q_j's are distinct and simple, the residue for the j^{th} root is found from equation IV-83.

$$\rho_{j,n} = \lim_{\substack{z\to q_j\\ \alpha\to\alpha_j}} \frac{N(z)}{\frac{d}{dz}D(z)} \qquad \text{(IV-137)}$$

where, for this problem,

$$N(z) = \frac{z^n H[\cos(S-m)\alpha]}{(z-1)(\gamma z+1-\gamma)} = \frac{z^n H[\cos(S-m)\alpha][1+2r\gamma(1-\cos\alpha)]^2}{2r(\cos\alpha-1)} \qquad \text{(IV-138)}$$

$$D(z) = H\cos S\alpha - S\sin S\alpha \sin\alpha \qquad \text{(IV-139)}$$

$$\frac{d}{dz}D(z) = \frac{S[H\sin S\alpha + S\sin\alpha\cos S\alpha + \sin S\alpha\cos\alpha][1+2r\gamma(1-\cos\alpha)]^2}{2r\sin\alpha} \qquad \text{(IV-140)}$$

The second equality for $N(z)$ comes from the relationship of $(z-1)$ and α, equation IV-118. The residue becomes then

$$\rho_{j,n} = \frac{H(\sin\alpha_j)[\cos(S-m)\alpha_j](q_j^n)}{S[1-\cos\alpha_j][(H\cos\alpha_j)(\sin S\alpha_j)+(S)(\sin\alpha_j)(\cos S\alpha_j)]} \qquad \text{(IV-141)}$$

or, after simplification using a trigonometric identity:

$$\rho_{j,n} = \frac{-H[\cos(S-m)\alpha_j][q_j^n]}{S\left[\tan\frac{\alpha_j}{2}\right]\left[(H\cos\alpha_j)(\sin S\alpha_j)+(S)(\sin\alpha_j)(\cos S\alpha_j)\right]} \qquad \text{(IV-142)}$$

Before summing over residues to find the solution, the assumption of distinct q_j's must be investigated. Study of the transcendental characteristic equation IV-135 shows that $(S+1)$ q_j's are real and distinct if the range of real α's is restricted from 0 to π and that one α_j is complex of the form $[\pi + \sqrt{-1}\,\phi(\alpha)]$. If the S real α_j's satisfy the equation, both $-\alpha_j$ and $(\alpha_j \pm p2\pi)$ also satisfy the equation. However, if two different α_j's are used that give the same q_j they have identical eigenvectors. This is seen as the m^{th} element in the j^{th} eigenvector

is given by $[\cos(S-m)\alpha_j]$; but from trigonometry we have

$$\cos(S-m)(\alpha_j) = \cos(S-m)(-\alpha_j) \qquad m = 0, 1, 2, \ldots, S \qquad \text{(IV-143)}$$

$$\cos(S-m)(\alpha_j) = \cos(S-m)(\alpha_j + p2\pi) \qquad \text{(IV-144)}$$

Thus, to have a matrix of eigenvectors which is non-singular, as required from matrix arguments, the q_j's must be distinct and the real α_j's are conveniently selected as those in the range 0 to π. Analogous arguments apply for the complex α. Thus we have (S+1) roots α_j's, S of which are real and fall between 0 and π and one of which is complex of the form $[\pi + \sqrt{-1}\,\phi(\alpha)]$ which result in (S+1) real, distinct q_j's.

Now, summing over all residues, the complete difference solution is

$$t_{m,n} = 1 - \frac{H}{S} \sum_{j=1}^{S+1} \frac{[\cos(S-m)\alpha_j][q_j^{n-}]}{\left[\tan\frac{\alpha_j}{2}\right]\left[(H+\cos\alpha_j)(\sin S\alpha_j)+(S)(\sin\alpha_j)(\cos S\alpha_j)\right]} \qquad \text{(IV-145)}$$

where the q_j's are given by equation IV-136 and the α_j's are the roots of equation IV-135. From equations IV-145 and II-53 and II-56, the analog solution is given by

$$t_{m,n} = 1 - \frac{H}{S} \sum_{j=1}^{S+1} \frac{[\cos(S-m)\alpha_j]\left[e^{-2S^2(1-\cos\alpha_j)\tau}\right]}{\left[\tan\frac{\alpha_j}{2}\right]\left[(H+\cos\alpha_j)(\sin S\alpha_j) + S\sin\alpha_j \cos S\alpha_j\right]} \qquad \text{(IV-146)}$$

Reviewing, the difference and analog solutions above are for using method G to approximate the continuous problem for a slab of width L, initially at zero temperature throughout with the right boundary insulated and the left boundary brought into contact with a fluid at unit temperature and heat transfer-coefficient h. In terms of dimensionless variables

$$\frac{\partial T}{\partial \tau} = \frac{\partial^2 T}{\partial \xi^2} \qquad 0 \le \xi \le 1 \qquad \text{(IV-147)}$$

Initial Condition:

$$T(\xi, 0) = 0 \qquad 0 \le \xi \le 1 \qquad \tau = 0 \qquad \text{(IV-148)}$$

Boundary Conditions:

$$H[T(0,\tau)-1] = \frac{\partial T}{\partial \xi}(0,\tau) \qquad \xi = 0 \qquad \tau \ge 0 \qquad \text{(IV-149)}$$

$$\frac{\partial T}{\partial \xi}(1,\tau) = 0 \qquad \xi = 1 \qquad \tau \ge 0 \qquad \text{(IV-150)}$$

The exact solution of the continuous problem is:

$$T(\xi,\tau) = 1 - 2H \sum_{j=0}^{\infty} \frac{[\cos(1-\xi)\nu_j]\left[e^{-\nu_j^2 \tau}\right]}{(\nu_j)[(H+1)(\sin\nu_j + \nu_j \cos\nu_j)]} \qquad \text{(IV-151)}$$

where the υ_j are defined by the characteristic equation,

$$\upsilon_j \tan \upsilon_j = H = \frac{hL}{k} \tag{IV-152}$$

The form of both the difference approximation and the continuous solution are the same; as a matter of fact, the continuous solution could be derived from the difference solution by properly taking limits as $S \to \infty$, $\Delta\xi \to 0$, and $\Delta\tau \to 0$. For a direct comparison, the only modification necessary is to substitute difference parameters for the continuous ξ, τ, and υ according to:

$$\psi = \upsilon \Delta\xi = \frac{\upsilon}{S} \tag{IV-153}$$

$$\frac{1}{S} = \Delta\xi \tag{IV-154}$$

$$\xi = m\Delta\xi \tag{IV-155}$$

$$\tau = n\Delta\tau \tag{IV-156}$$

$$r = \frac{\Delta\tau}{(\Delta\xi)^2} \tag{IV-157}$$

which then allows us to write all the solutions in difference form.

Difference Solution:

$$t_{m,n} = 1 - \frac{H}{S} \sum_{j=1}^{S+1} \frac{[\cos(S-m)\alpha_j]\left[\frac{1-2r(1-\gamma)(1-\cos\alpha_j)}{1+2r\gamma(1-\cos\alpha_j)}\right]^n}{\left[\tan\frac{\alpha_j}{2}\right]\left[H+\cos\alpha_j)(\sin S\alpha_j) + S(\sin\alpha_j)(\cos S\alpha_j)\right]} \tag{IV-158}$$

Analog Solution:

$$t_{m,n} = 1 - \frac{H}{S} \sum_{j=1}^{S+1} \frac{\left[\cos(S-m)\alpha_j\right]\left[e^{-2r(1-\cos\alpha_j)}\right]^n}{\left[\tan\frac{\alpha_j}{2}\right]\left[H+\cos\alpha_j)(\sin S\alpha_j)+ S(\sin\alpha_j)(\cos S\alpha_j)\right]} \tag{IV-159}$$

where α_j is defined by

$$S(\sin\alpha_j)(\tan S\alpha_j) = H \qquad j = 1, 2, \ldots, S+1 \tag{IV-160}$$

Continuous Solution:

$$T(m,n) = 1 - 2H \sum_{j=1}^{\infty} \frac{\left[\cos(S-m)\psi_j\right]\left[e^{-\psi_j^2 r}\right]^n}{(S\psi_j)\left[H+\cos\psi_j)(\sin S\psi_j) + S\psi_j(\cos S\psi_j)\right]} \tag{IV-161}$$

where

$$S\psi_j(\tan S\psi_j) = H \qquad j = 1, 2, \ldots, \infty \tag{IV-162}$$

Thus, the z-transform leads to results which allow a comparison of the analytic solution of the difference formulation with the continuous solution. The above equations are scalar representations of the m^{th} component* of the vector solution derived before. The particular solution

* As this method is based on mesh $\Delta\xi$, m starts at zero instead of 1 as it should in conventional matrix-vector nomenclature. The m^{th} component of the vector is then the temperature at point m_{th} which in conventional vector notation is the (m+1) component; the m^{th} row of the eigenvector matrix consists of the coefficients in the matrix row that are

vector for all solutions has dimension (S+1) with a one for each element. The eigenvector matrix for the difference and analog solution has an element in the m^{th} row* and j^{th} column defined by $[\cos (S-m)\alpha_j]$ and the corresponding element in the continuous solution is defined by $[\cos (S-m)\psi_j]$. The j^{th} element of the initial vector, or vector of Fourier coefficients, is, for the approximate solutions, $H/S(\tan \frac{\alpha_j}{2})[(H+\cos\alpha_j)(\sin S\alpha_j)+ S(\sin\alpha_j)(\cos S\alpha_j)]$, and for the continuous solution, $2H/(S\psi_j)[(H+\cos\psi_j)(\sin S\psi_j)+S\psi_j(\cos S\psi_j)]$. The characteristic equations that define the α_j and ψ_j are given by equations IV-160 and IV-162.

Another method of comparison of the solutions that would apparently avoid the lengthy inversion procedure would be to derive the z-transforms of the analog and continuous solutions and compare them to the z-transform of the difference solution. However, to convert the Laplace transform to a z-transform also requires a complex integration. Most chemical engineers (including the author) would have difficulty comparing the meaning of the transforms.

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* (continued)
in the equation for the m^{th} point, which is the (m+1) row in conventional matrix notation. A similarcomment applies if method C is being discussed as m starts at $\frac{1}{2}$ and the m^{th} component would be the $(m+\frac{1}{2})$ component in conventional matrix notation.

2. Problem I, Averaged Method G--Ramp-Step Equivalence.

For problems with certain types of initial temperature distributions, a backward-averaged solution is identical to that obtained by replacing a constant fluid temperature with a ramp-step fluid temperature function, as shown previously.

The solution for method G applied to problem I using the ramp-step function will now be found. The ramp-step function for this problem is given by equation IV-54, and is

$$t_{f,n} = \begin{cases} \frac{1}{2} & n=0 \\ 1 & n \geq 1 \end{cases} \qquad \text{(IV-163)}$$

To generalize this for implicit methods, we use the fluid temperature from equation IV-163 above directly and do not use the weights of γ and $(1-\gamma)$ as shown in equation IV-94. The z-transform for equation IV-163 is easily derived from the series definition, equation IV-67.

$$\mathcal{Z}\{t_{f,n}\} = \tfrac{1}{2}\, z^{-0} + z^{-1} + z^{-2} + \ldots + z^{-n} + \ldots$$

$$= \tfrac{1}{2} + \sum_{n=1}^{\infty} z^{-n} = \tfrac{1}{2} - 1 + \sum_{n=0}^{\infty} z^{-n} \qquad \text{(IV-164)}$$

$$= \frac{z}{z-1} - \tfrac{1}{2} = \frac{z+1}{2(z-1)}$$

To derive the solution using this "ramp-step" function instead of a true step, the transformed partial difference equation IV-112 and the

adiabatic boundary condition equation IV-114 apply if a zero initial condition is assumed throughout. The boundary condition represented by equation IV-113 is modified by the substitution of equation IV-164 for $\bar{t}_f$ and ignoring the γ weighting for $\bar{t}_f$ (γ set to zero when it is a coefficient of $\bar{t}_{f,0}$):

$$\left[z-1+2r\left(1+\frac{H}{S}\right)(\gamma z+1-\gamma)\right]\bar{t}_0 - 2r(\gamma z+1-\gamma)\bar{t}_1 = \frac{2rH}{S}\left[\frac{z+1}{2(z-1)}\right] \qquad \text{(IV-165)}$$

Since the transformed partial difference equation and adiabatic boundary condition are unchanged, the solution for these two equations is written directly,

$$\bar{t}_m = \frac{P\cos(S-m)\alpha}{\cos S\alpha} \qquad \text{(IV-166)}$$

Using the previous procedure of substituting $\bar{t}_0$ and $\bar{t}_1$ as found from equation IV-166 into equation IV-165 and solving for $(P/\cos S\alpha)$, we find that

$$\bar{t}_m = \left[\frac{z+1}{2(z-1)}\right]\left[\frac{H\cos(S-m)\alpha}{(\gamma z+1-\gamma)\left\{H\cos S\alpha - S\sin\alpha\sin S\alpha\right\}}\right] \qquad \text{(IV-167)}$$

(This equation could be found directly by substituting equation IV-146 for $\bar{t}_f$ into equation IV-129, ignoring γ.)

This transform is the average of the transform for the true step function and that transform divided by z. Further, as $\bar{t}_m$ goes to a constant value as z goes to zero, $\bar{t}_m$ contains neither a pole nor zero at zero.

According to the previous discussion, a simple pole at zero is introduced when multiplying by z^{n-1}; and in order that the solution fit the initial conditions, it must be included. Further, by comparison of equation IV-167 with the previous transform, equation IV-131, the solution is found to be the average of the result for n and for (n-1) in addition to the residue of the zero singularity.

$$t_{m,n} = \tfrac{1}{2}\left\{2 - \frac{H}{S}\sum_{j=1}^{S+1} \frac{\left[1+\frac{1}{q_j}\right]\left[\cos(S-m)\alpha_j\right]\left[q_j\right]^n}{\left[\tan\frac{\alpha_j}{2}\right]\left[(H+\cos\alpha_j)(\sin S\alpha_j)+S\sin\alpha_j\cos S\alpha_j\right]}\right\} \qquad \text{(IV-168)}$$

$$-\tfrac{1}{2}\left\{\frac{[H\cos(S-m)\beta][0]^n}{[H\cos S\beta - S(\sin\beta)(\sin S\beta)][1-\gamma]}\right\}$$

$$m = 0, 1, \ldots, S$$

$$n \geq 0$$

where the q_j's and α_j are as defined previously by equations IV-136 and IV-160, respectively, and

$$\cos\beta = \frac{2r(1-\gamma)-1}{2r(1-\gamma)} \qquad \text{(IV-169)}$$

The solution equation IV-168 applies for all values of γ including a γ of 1, even though $(\cos\beta)$ becomes infinite for a γ of 1. The argument used previously to show that the term $(\gamma z+1-\gamma)$ in the transform in equation IV-131 does not give a pole can be used here to show that the β term has a finite limit for all values of γ including a value of

one. The necessity for adding the zero root is obvious, as a comparison of this solution, equation IV-168, with the previous one, equation IV-158, shows that if the first meets the initial conditions the second cannot unless another term is added. The above result has been checked numerically to make sure it does fit the initial condition. Since, as mentioned before, the zero root only gives a contribution for n of zero, we may neglect it in comparing the results. The effect of using the "ramp-step" is then essentially an averaging process; that is, the same results could be obtained by stepping out the solution with a true step and averaging the results at n and $(n-1)$ and using this average at n. This is an alternate proof of the relationship between averaged methods and the ramp-step replacement for a step change in fluid temperature. The factor $(1+1/q_j)$ actually modifies the Fourier coefficients in the initial vector and further studies would be required to determine any improvement in accuracy.

3. Problem II, Infinite H, Method G

For the case of infinite heat-transfer coefficient with a zero initial condition and a boundary at unity,

$$t_{m,0} = \delta_{m,0} \tag{IV-170}$$

The transformed partial difference equation IV-117 is no longer homogeneous; substituting for $t_{m+1,0}$, $t_{m,0}$, and $t_{m-1,0}$ from

equation IV-170 into equation IV-101 together with equation IV-115, and noting that $t_{m+1,0}$ and $t_{m,0}$ are zero for the range of m's used, this equation is:

$$\bar{t}_{m-1} - 2\cos\alpha\,\bar{t}_m + \bar{t}_{m+1} = \left[\frac{z\gamma}{(\gamma z+1-\gamma)}\right]\left[\delta_{m-1,0}\right] \qquad \text{(IV-171)}$$

$$m = 1, 2, \ldots, S$$

and the left boundary condition is

$$t_{0,n} = t_{f,n} \qquad \text{(IV-172)}$$

and the transformed conditions are:

$$\bar{t}_0 = \frac{z}{z-1} \qquad \text{(IV-173)}$$

$$\bar{t}_{S+1} = \bar{t}_{S-1} \qquad \text{(IV-174)}$$

Assuming the particular solution is of the form,

$$\bar{t}_{m,P} = F\,\delta_{m,0} \qquad \text{(IV-175)}$$

substituting into equation IV-171 according to the method of undetermined parameters:

$$F\,\delta_{m-1,0} - 2F\,\delta_{m,0}\cos\alpha + F\,\delta_{m+1,0} = \left(\frac{z\gamma}{\gamma z+1-\gamma}\right)\delta_{m-1,0} \qquad \text{(IV-176)}$$

$$m = 1, 2, \ldots, S$$

or, as $\delta_{m,0}$ and $\delta_{m+1,0}$ are zero for the m's used,

$$F = \left[\frac{z\gamma}{z\gamma+1-\gamma}\right] \tag{IV-177}$$

and

$$\bar{t}_m = P \cos m\alpha + G \sin m\alpha + \frac{z\gamma\delta_{m,0}}{[z\gamma+1-\gamma]} \tag{IV-178}$$

$$m = 0, 1, \ldots, S, S+1$$

Solving for P and G according to the previous procedure gives the complete transformed difference temperature as,

$$\bar{t}_m = \frac{z}{z-1}\left[\frac{\cos(S-m)\alpha}{(z\gamma+1-\gamma)(\cos S\alpha)}\right] + \frac{z\gamma\,\delta_{m,0}}{(z\gamma+1-\gamma)} \tag{IV-179}$$

$$m = 0, 1, \ldots, S+1$$

This is not the transform that would be obtained by taking limits of equation IV-131 as H or h goes to infinity; because of the change in initial conditions, the term involving the Kronecker delta function is added. However, the "main" transform could be found by taking limits.

Inversion may be carried out as before. The first term has simple poles at

$$z = 1 \tag{IV-180}$$

and at

$$z = q_j = \frac{1-2r(1-\gamma)(1-\cos\alpha_j)}{1+2r(1-\gamma)(1-\cos\alpha_j)} \qquad \text{(IV-181)}$$

$$j = 0, \ldots, S-1$$

where α_j are the roots of

$$\cos S\alpha_j = 0 \qquad \text{(IV-182)}$$

or

$$\alpha_j = \frac{(2j+1)\pi}{2S} \qquad j = 0, \ldots, S-1 \qquad \text{(IV-183)}$$

Note that because $t_{0,n}$ is fixed there is one less degree of freedom, thus one less q_j and α_j. (The complex α_j fortunately is eliminated.) Now considering the pole in the first term at $(\gamma-1)/\gamma$, and using arguments like those for the case of finite h, we conclude that a zero exists at $z = (\gamma-1)/\gamma$ of the order of $(m-1)$. Consequently, only for an m of zero is there a simple pole at $(\gamma-1)/\gamma$, or, equivalently, only for an m of zero does this pole have a non-zero residue. However, its residue is the negative of the residue of the second term of the transform. Thus, this pole gives no contribution to the solution. Evaluating and summing the residues for the other poles we obtain (after trigonometric simplification)

$$t_{m,n} = 1 - \frac{1}{S} \sum_{j=0}^{S-1} \left[\frac{1}{\tan\frac{\alpha_j}{2}} \right] \left[\sin m\alpha_j \right] \left[\frac{1-2r(1-\gamma)(1-\cos\alpha_j)}{1+2r\gamma(1-\cos\alpha_j)} \right]^n \qquad \text{(IV-184)}$$

where

$$\alpha_j = \frac{(2j+1)\pi}{2S} \tag{IV-185}$$

This result could have been obtained by taking the limit of equations IV-158 and IV-160, the characteristic and the solution equations, as H goes to infinity even though the transform might not be found correctly by taking limits. The solution is identical to that reported in O'Brien et al. (2) for the same problem solved by von Neumann's Method and a finite Fourier harmonic analysis. The eigenvectors and eigenvalues reported agree with the results from many workers (15, 10, 21, 17, 29, 22, 2, 3, 23, 24, 4, 30) as derived by separation of variables technique or matrix analysis.

4. Problem V, Semi-Infinite Solid, Method G--Branch Cut Singularity

The last type of example solution carried out here is that of applying method G to a semi-infinite solid, whose left boundary temperature is specified as unity and which extends to infinity in the ξ direction. The initial condition is taken as zero. Since an implicit method would require the solution of an infinite number of equations only the explicit case is considered. The transformed partial difference equation is then

$$\bar{t}_{m-1} - 2\cos\alpha\bar{t}_m + \bar{t}_{m+1} = 0 \tag{IV-186}$$

where

$$\cos\alpha = \frac{z-1+2r}{2r} \qquad m = 1, 2, \ldots, \infty \qquad \text{(IV-187)}$$

The transformed boundary conditions are:

$$\bar{t}_0 = \frac{z}{z-1} \qquad \text{(IV-188)}$$

$$\bar{t}_\infty = 0 \qquad \text{(IV-189)}$$

Assuming that the solution to the partial difference equation is equation IV-120 P and G may be determined from the above boundary equation giving

$$\bar{t}_m = \frac{z}{z-1}\left[e^{-m\alpha\sqrt{-1}}\right] \qquad \text{(IV-190)}$$

From complex variable theory the formula for the inverse cosine may be written:

$$\alpha = \cos^{-1}\left(\frac{z-1+2r}{2r}\right) = -\sqrt{-1}\ln\left[\frac{z-1+2r}{2r} + \sqrt{\left(\frac{z-1+2r}{2r}\right)^2 - 1}\right] \qquad \text{(IV-191)}$$

Substituting this into equation IV-190 and simplifying, we have,

$$\bar{t}_m = \frac{z}{z-1}\left[\frac{2r}{z-1+2r+\sqrt{(z-1)(z-1+4r)}}\right]^m \qquad \text{(IV-192)}$$

This function has, in addition to the pole at +1, a branch cut from (1-4r) to +1 on the real axis because of the square root of the two

factors (28). To invert the transform we integrate $z^{n-1}\,\bar{t}_m$ along a dumbbell-shaped contour in the z-plane. This contour is shown in Figure IV-5(b) for $r = \frac{1}{2}$; and the direction is counter-clockwise about the closed dumbbell indicated by the dashed line. (Actually the inversion integral is along ABC; but as $z^{n-1}\,\bar{t}$ is analytic within ABCDA, the inversion integral may be shown to be equal to that found by going counter-clockwise around the dumbbell.) The integrals are evaluated allowing the radius of the circles δ and distance from the real axis ϵ to go to zero.

The path around the pole and branch point +1 is given by

$$\Gamma_1 \qquad z = 1 + \delta e^{\sqrt{-1}\,\varphi_1} \qquad -\pi \le \varphi_1 \le \pi \tag{IV-193}$$

where φ_1 is allowed to vary from $-\pi$ to π. Substituting this into the transform and taking the limit and integrating we obtain

$$J_1 = \lim_{\delta \to 0} \int_{\Gamma_1} z^{n-1}\,\bar{t}_m\,dz = 2\pi\sqrt{-1} \tag{IV-194}$$

The path around the branch point at (1-4r) is

$$\Gamma_3 \qquad z = 1 + \delta e^{\sqrt{-1}\,\varphi_2} \qquad 0 \le \varphi_2 \le 2\pi \tag{IV-195}$$

Substituting and carrying out the integration gives

$$J_3 = \lim_{\delta \to 0} \int_{\Gamma_3} z^{n-1}\,\bar{t}_m\,dz = 0 \tag{IV-196}$$

The path for the line above the real axis is

$$\Gamma_2 \qquad z = x + \sqrt{-1}\,\epsilon \tag{IV-197}$$

and below is

$$\Gamma_4 \qquad z = x - \sqrt{-1}\,\epsilon \tag{IV-198}$$

After making the above substitutions and taking the required limits, the integrals for Γ_2 and Γ_4 may be combined. The result is, after simplification and trigonometric substitution:

$$J_2 + J_4 = \lim_{\epsilon \to 0} \int_{\Gamma_2+\Gamma_4} z^{n-1} \bar{t}_m \, dz = 2\sqrt{-1} \int_0^{\pi} \frac{(\sin m)[1-2r(1-\cos\alpha)]^n \, d\alpha}{\tan\frac{\alpha}{2}} \tag{IV-199}$$

The actual integrations are not shown as they involve a considerable amount of algebra, and are straightforward after the limits are taken. The inverse transform is $(1/2\pi\sqrt{-1})$ times the sum of the integrals:

$$t_{m,n} = 1 - \frac{1}{\pi} \int_0^{\pi} \frac{(\sin m)[1-2r(1-\cos\alpha)]^n \, d\alpha}{\tan\frac{\alpha}{2}} \tag{IV-200}$$

This result could be obtained from equations IV-184 and IV-185 by letting S go to infinity without $\Delta\xi$ going to zero. Briefly let

$$\alpha = \alpha_0 + j\Delta\alpha$$

$$\text{where } \alpha_0 = \pi/2S \tag{IV-201}$$

$$\text{and } \Delta\alpha = \pi/S$$

Now, noting from the characteristic equation IV-182 that as S goes to infinity any value of α between 0 and π satisfies the equation, or, equivalently, α becomes continuous, and taking limits on the above equations, we have

$$\lim_{S \to 0} \alpha_0 = 0 \qquad \text{(IV-202)}$$

$$\lim_{S \to \infty} \frac{1}{S} = \lim_{S \to \infty} \frac{\Delta\alpha}{\pi} = \frac{d\alpha}{\pi} \qquad \text{(IV-203)}$$

Substituting for the limit of 1/S and changing the sum to an integral we obtain the above result.

5. Conclusions

Most of the results presented and compared in following subsections were derived using the principles, techniques, and manipulations shown in deriving the previous results. The only major difference for methods using mesh $\Delta\xi/2$ is that the m's are 1/2, 3/2, ... S-1/2 for convenience in derivation and in comparisons; no other complications appear.

The z-transform method for solving partial difference equations was demonstrated above by finding the analytic solution for the difference approximation of the one-dimensional diffusion equation for several types of boundary and initial conditions. These analytic difference solutions are of the same form as the solution of the differential equation; thus, comparisons between the continuous solution and difference

approximations are readily possible. The z-transform method suffers the same restrictions as the Laplace transform method, and thus the difference solutions can be derived only for those cases where the continuous solution can be found. This is not a disadvantage in comparing several approximate methods to the exact continuous solution.

The z-transform technique has several advantages over the other methods for solving partial difference equations. It is a methodical procedure mostly consisting of algebraic manipulations that allow one to find the complete solution to the difference problem. The only "trick" in determining the solution is the substitution of α (equation IV-115); but all the other methods require this or an equivalent substitution also. This substitution is suggested by a form of the solution of the ordinary difference equation, if it is not made. The procedure has the advantage that it gives the particular or quasi-steady-state solution and the Fourier coefficients in the initial vector, in addition to the eigenvectors and eigenvalues. As demonstrated in the next subsection, the Fourier coefficient in the initial vector is one of the most important quantities in obtaining accurate approximations. The direct matrix method requires significant additional work just to determine the analytic expressions for the eigenvectors after the eigenvalues are found. The separation of variables technique determines the eigenvectors and eigenvalues in a way very much like that for the z-transform method. Even after these two quantities are found, the particular or quasi-

steady-state solution must be found. And possibly the most difficult step with these more conventional techniques is to determine the coefficients that fit the eigenvectors to the initial condition. This requires determining the orthogonality relationships and the analytic evaluation of a series of finite sums.

No rigorous proof has been presented that the z-transform solution of a partial difference equation is the same as the eigenvector-eigenvalue problem. Indeed, no proof has been presented that z-transforms are applicable to partial difference equations. However, the basis for the z-transforms has been presented and no mathematical inconsistency seems to have been introduced in applying them to the partial difference equations. The difference solutions derived have been compared with published results derived by other methods and in each case the transform results are identically the same for quantities that other researchers have obtained. Usually this is restricted to a comparison of the eigenvalues and sometimes eigenvectors for the case of infinite heat-transfer coefficient. The only comparison for a complete solution including the initial vector and particular solution was mentioned previously. Further, almost all of the results have been checked numerically. That is, the difference solution has been computed for fixed values of S, r, and γ, by stepping out the solution and from the z-transform solution. In all cases (after algebraic and numerical errors were removed) the two solutions checked except

for discrepancies which could be accounted for by round-off error (usually four-digit accuracy). Thus, the z-transform method is concluded to be a valid, useful procedure for studying the one-dimensional partial difference equation of diffusion.

In addition to the type of problems studied and compared here, there are many other applications where this method should be useful. Already it has been successfully applied to Richardson's (2) unstable explicit three-level approximation to the diffusion equation, where the temperature-time derivative is replaced with $(t_{m,n+1} - t_{m,n-1})/2\Delta\tau$ instead of the two-level formula used above. The other main application to the diffusion equation is to solve its partial difference equation for the radial direction in either cylindrical or spherical coordinates. Preliminary attempts to derive this solution for the radial coordinate in cylindrical coordinates have not been successful, but, in this author's opinion, this was caused by an inability to find the substitution equivalent to the relationship between z and α that gives simplification to the transformed difference equation. This in turn is caused by not having a sufficient familiarity with Bessel functions and their identities.

In addition to the study of the approximate methods for the diffusion equation, z-transforms should be of use in studying approximate methods for other equations which lead to a linear partial difference equation of an initial-value type with linear boundary conditions for which the exact solution may be found by the Laplace transform.

Specifically, two partial differential equations for which approximate solution methods might be studied are the wave equation and the equation governing transient bending of beams. The form of these are, respectively,

$$\frac{\partial^2 y}{\partial \theta^2} = \frac{\partial^2 y}{\partial x^2} \tag{IV-204}$$

and

$$\frac{EI}{m} \frac{\partial^4 y}{\partial x^4} + \frac{\partial^2 y}{\partial \theta^2} = 0 \tag{IV-205}$$

where $\frac{EI}{m}$ = flexural rigidity.