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Donald M. Curry
Lyndon B. Johnson Space Center
Houston, Texas 77058

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A COMPARISON OF IMPLICIT NUMERICAL METHODS FOR SOLVING THE TRANSIENT SPHERICAL DIFFUSION EQUATION

By Donald M. Curry
Lyndon B. Johnson Space Center

SUMMARY

Comparative numerical temperature results obtained by using two implicit finite-difference procedures for the solution of the transient spherical heat-conduction equation are presented. The strongly implicit procedure is compared to the more standard alternating-direction implicit procedure by using a two-dimensional solid spherical model. The numerically generated temperature results obtained by using the strongly implicit procedure and the alternating-direction implicit procedure are compared with exact solutions to assess the relative accuracy and efficiency of the two numerical methods. Special attention was given to the solution in the regions of singularities associated with the governing partial differential equation. For the examples solved, the numerical results obtained by a modified version of the strongly implicit procedure and by the alternating-direction implicit procedure are in close agreement with the exact solution.

INTRODUCTION

Numerous authors have discussed the various numerical methods available for solving the transient diffusion equation. Solutions to the diffusion equation by means of numerical methods are required for a wide variety of design/development problems associated with the aerospace, petroleum, and chemical industries.

Trent and Welty (ref. 1) presented a good summary of numerical methods for solving transient-heat-conduction problems. However, they did not include discussion of a recently developed iterative technique (Stone, ref. 2) called the strongly implicit procedure (SIP). The SIP was shown to have several advantages over other implicit numerical techniques in solving large sets of algebraic equations that arise in the approximate solution of multidimensional partial differential equations. Weinstein et al. (ref. 3) have used the SIP successfully to solve systems of equations arising in multiphase, two-dimensional reservoir flow problems. The SIP has been used by Curry (ref. 4) in the solution of two-dimensional heat and mass transfer in porous media. Steen and Ali (ref. 5) compared the SIP algorithm with the more conventional implicit method in the solution of the nonlinear partial differential equation for the flow of a real gas in two dimensions. However, few two-dimensional numerical solutions of the transient-heat-conduction equation for both spherical and cylindrical coordinates can be found in the literature. Albasiny (ref. 6) presented an implicit numerical solution for a cylindrical heat-conduction problem, including the effects of the singularity at the center of the solid. Kee (ref. 7) developed a finite-difference algorithm for the diffusion equation for a solid sphere.

In this report, the SIP is compared with the more conventional alternating-direction implicit procedure (ADIP) (ref. 8) by using a two-dimensional spherical heat-conduction model. The temperature results obtained are compared to exact solutions of the spherical heat-conduction equation for various boundary conditions. Attention is given to the adequacy of the finite-difference representation in the neighborhood of the singularities located at the geometrical center, $r = 0$, and along the boundaries, $\phi = 0, \pi$.

SYMBOLS

A, B, C, D, E, Q	parameters known from previous time level and previous iteration
C_p	specific heat
k	thermal conductivity
m, n	iterative variables used in equation (14)
q'''	volumetric heat source (sink)
R	outer sphere radius
T	temperature
T'	unknown temperature in difference equations
t	time
r, ϕ, θ	spherical space coordinates
x, y	rectangular space coordinates
γ	iteration parameter
ρ	density

Subscripts

i	ϕ-direction node location
j	r-direction node location
x	x-direction
y	y-direction

Superscript

'	indicates parameter at next time step or iteration

THEORETICAL MODEL

The transient-heat-conduction equation in spherical coordinates, with the assumption of constant thermophysical properties, is given as

$$\rho C_p \frac{\partial T}{\partial t} = k \left[\frac{1}{r} \frac{\partial^2 (rT)}{\partial r^2} + \frac{1}{r^2 \sin \phi} \frac{\partial}{\partial \phi}\left(\sin \phi \frac{\partial T}{\partial \phi}\right) + \frac{1}{r^2 \sin^2 \phi} \frac{\partial^2 T}{\partial \theta^2}\right] + q''' \qquad (1)$$

where ρ is density; r, ϕ, and θ are spherical space coordinates, defined in figure 1; T is temperature; t is time; k is thermal conductivity; C_p is specific heat; and q''' is volumetric heat source.

If the temperature field has azimuthal symmetry, then

$$\frac{\partial^2 T}{\partial \theta^2} = 0 \qquad (2)$$

Equation (1) can then be written in two dimensions as

$$\rho C_p \frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial r^2} + \frac{2k}{r} \frac{\partial T}{\partial r} + \frac{k}{r^2 \sin \phi} \frac{\partial}{\partial \phi}\left(\sin \phi \frac{\partial T}{\partial \phi}\right) + q''' \qquad (3)$$

This two-dimensional unsteady heat conduction in the spherical domain is bounded by

$$0 \leq r \leq R$$

and

$$0 \leq \phi \leq \pi$$

with the boundary and initial conditions as

$$T(R, \phi, t) = f_1(\phi, t) \tag{4}$$

where R is the outer sphere radius.

In formulating the boundary conditions, it should be noted that equation (3) is singular at $r = 0$ and for $\phi = 0, \pi$. The boundary condition represented by equation (4) permits a sphere with a variable surface temperature from $\phi = 0$ to $\phi = \pi$ (i.e., a sphere that is hot at the top and cold at the bottom). This variation obviously will result in a temperature gradient at $r = 0$. For this analysis, it is assumed that

$$\frac{\partial T}{\partial r} = 0, \quad r = 0 \tag{5}$$

Equation (5) is strictly true only on $\phi = \pi/2$.[1]

On the assumption of symmetry along $\phi = 0, \pi$, then

$$\frac{\partial T}{\partial \phi} = 0, \quad \phi = 0, \pi \tag{6}$$

The initial condition is

$$T(r, \phi, 0) = f_2(r, \phi) \tag{7}$$

Equations (3) through (7) are the governing relations used in this investigation of the SIP and ADIP numerical procedures.

---

[1]This assumption of $\partial T/\partial r = 0$, $r = 0$, for all ϕ values will be discussed in a subsequent section of this report.

When the sphere is solid rather than hollow, a singularity exists at $r = 0$. At $r = 0$, the terms

$$\frac{2k}{r} \frac{\partial T}{\partial r} \quad \text{and} \quad \frac{k}{r^2 \sin \phi} \frac{\partial}{\partial \phi} \left(\sin \phi \frac{\partial T}{\partial \phi} \right)$$

are indeterminate. These terms can be evaluated by using L'Hospital's rule (ref. 9),[2]

$$\lim_{r \to 0} \frac{2k}{r} \frac{\partial T}{\partial r} = \lim_{r \to 0} \frac{2k \frac{\partial}{\partial r} \left(\frac{\partial T}{\partial r} \right)}{\frac{\partial}{\partial r}(r)} = 2k \frac{\partial^2 T}{\partial r^2}$$

and

$$\lim_{r \to 0} \frac{k}{r^2 \sin \phi} \frac{\partial}{\partial \phi} \left(\sin \phi \frac{\partial T}{\partial \phi} \right) = \lim_{r \to 0} \frac{\frac{\partial}{\partial r} \left[\frac{k}{\sin \phi} \frac{\partial}{\partial \phi} \left(\sin \phi \frac{\partial T}{\partial \phi} \right) \right]}{2r}$$

$$= \lim_{r \to 0} \frac{\frac{\partial^2}{\partial r^2} \left\{ \frac{k}{\sin \phi} \left[\frac{\partial}{\partial \theta} \left(\sin \phi \frac{\partial T}{\partial \phi} \right) \right] \right\}}{2} = 0$$

Likewise, a singularity exists at $\phi = 0, \pi$ in the term

$$\frac{k}{r^2 \sin \phi} \frac{\partial}{\partial \phi} \left(\sin \phi \frac{\partial T}{\partial \phi} \right)$$

---

[2] For the limits to exist, it is required that

$$\frac{1}{\sin \phi} \frac{\partial}{\partial \phi} \left(\sin \phi \frac{\partial T}{\partial \phi} \right) = 0, \quad r = 0$$

$$\frac{\partial}{\partial r} \left[\frac{1}{\sin \phi} \frac{\partial}{\partial \phi} \left(\sin \phi \frac{\partial T}{\partial \phi} \right) \right] = 0, \quad r = 0$$

Application of L'Hospital's rule to this term yields

$$\lim_{\phi\to 0,\ \pi}\left[\frac{k}{r^2\sin\phi}\frac{\partial}{\partial\phi}\left(\sin\phi\,\frac{\partial T}{\partial\phi}\right)\right] = \lim_{\substack{\phi\to 0\\ \phi\to\pi}} \frac{\frac{\partial}{\partial\phi}\left[\frac{k}{r^2}\frac{\partial}{\partial\phi}\left(\sin\phi\,\frac{\partial T}{\partial\phi}\right)\right]}{\frac{\partial}{\partial\phi}(\sin\phi)}$$

$$= \frac{2k}{r^2}\frac{\partial^2 T}{\partial\phi^2}$$

Therefore, at the singularities,

$$\frac{2k}{r}\frac{\partial T}{\partial r} = 2k\,\frac{\partial^2 T}{\partial r^2},\quad r = 0 \tag{8a}$$

$$\frac{k}{r^2\sin\phi}\frac{\partial}{\partial\phi}\left(\sin\phi\,\frac{\partial T}{\partial\phi}\right) = 0,\quad r = 0 \tag{8b}$$

and

$$\frac{k}{r^2\sin\phi}\frac{\partial}{\partial\phi}\left(\sin\phi\,\frac{\partial T}{\partial\phi}\right) = \frac{2k}{r^2}\frac{\partial^2 T}{\partial\phi^2},\quad \phi = 0,\ \pi \tag{8c}$$

The singularity at $r = 0$ can also be eliminated by approximating the center in a Cartesian formulation.[3] This approach is discussed by Smith (ref. 10). A related question concerning a singularity for the cylindrical problem is discussed by Albasiny (ref. 6). A third method of eliminating the singularity at $r = 0$ is to simply assume that a small but finite radius exists at the center; i.e., hollow-sphere approximation. All three approaches were examined in this investigation and will be discussed in a subsequent section of this report.

[3]The singularities at $r = 0$ and $\phi = 0,\ \pi$ can also be eliminated by not specifying node points on the boundaries.

IMPLICIT DIFFERENCE EQUATION FORMULATION

Equation (3) describes the heat transfer within a spherical region, and a solution is achieved by approximating the partial derivatives with the use of suitable finite-difference expressions involving the independent and dependent variables. The two-dimensional spherical region with an r, ϕ grid system imposed is shown in figure 2. An implicit central-difference equation for each grid point (i, j) within the specified region can be written as

$$\rho C_p \left(\frac{T'_{i,j} - T_{i,j}}{\Delta t}\right) = k_{i,j}\left[\frac{T'_{i,j+1} - 2T'_{i,j} + T'_{i,j-1}}{(\Delta r)^2}\right] + \frac{2k_{i,j}}{r_{i,j}}\left(\frac{T'_{i,j+1} - T'_{i,j-1}}{2\,\Delta r}\right) + \frac{k_{i,j}}{r_{i,j}^2}\left[\frac{T'_{i+1,j} - 2T'_{i,j} + T'_{i-1,j}}{(\Delta\phi)^2}\right] + \frac{k_{i,j}\cos\phi_{i,j}}{r_{i,j}^2 \sin\phi_{i,j}}\left(\frac{T'_{i+1,j} - T'_{i-1,j}}{2\,\Delta\phi}\right) + q''' \tag{9}$$

where T' is the unknown temperature. Equation (9) can be written as

$$\left[\frac{k_{i,j}}{r_{i,j}^2(\Delta\phi)^2} + \frac{k_{i,j}\cos\phi_{i,j}}{r^2 \sin\phi_{i,j}(2\,\Delta\phi)}\right]T'_{i+1,j} + \left[\frac{k_{i,j}}{(\Delta r)^2} + \frac{k_{i,j}}{r_{i,j}\,\Delta r}\right]T'_{i,j+1} - \left[\frac{2k_{i,j}}{(\Delta r)^2} + \frac{2k_{i,j}}{r_{i,j}^2(\Delta\phi)^2} + \frac{\rho C_p}{\Delta t}\right]T'_{i,j} + \left[\frac{k_{i,j}}{r_{i,j}^2(\Delta\phi)^2} - \frac{k_{i,j}\cos\phi_{i,j}}{r_{i,j}^2\sin\phi_{i,j}\,(2\,\Delta\phi)}\right]T'_{i-1,j} + \left[\frac{k_{i,j}}{(\Delta r)^2} - \frac{k_{i,j}}{r_{i,j}\,\Delta r}\right]T'_{i,j-1} = -q'''_{i,j} - \frac{\rho C_p}{\Delta t}T_{i,j} \tag{10}$$

Rewriting equation (10) yields

$$A_{i,j}T'_{i,j-1} + B_{i,j}T'_{i-1,j} + C_{i,j}T'_{i,j} + D_{i,j}T'_{i+1,j} + E_{i,j}T'_{i,j+1} = Q_{i,j} \quad (11)$$

Equation (11) has five unknown temperatures per grid point (i,j). The values of A, B, C, D, E, and Q are known on the basis of the previous time level and/or the previous iteration. A set of equations similar to equation (11) can be written for all i,j grid points within the region and on the boundaries.[4] This matrix of equations can then be inverted to yield the unknowns, $T'_{i,j}$. For large systems of equations, this matrix solution can become very time consuming.

NUMERICAL SOLUTION TECHNIQUE

Stone (ref. 2) developed the SIP, an iterative method for solving sets of algebraic equations that occur for multidimensional systems. This method has been used successfully in solving problems involving two-dimensional, steady-state heat conduction, as well as multidimensional flow in a petroleum reservoir (ref. 3). The foundation of the SIP calculation method is based on the approximate factoring of the five-diagonal matrix (five nonzero elements in each row of matrix) generated by equation (11) into three-diagonal upper and lower triangular matrices. The detailed mathematical reduction process required to derive the upper and lower triangular matrices is presented by Stone (ref. 2). The equations used in the SIP algorithm to solve for the unknown variable $T'_{i,j}$, together with the boundary condition restrictions, can be found in references 2 and 3.

A second method used in the solution of equation (11) is the ADIP (Peaceman and Rachford (ref. 8)), which reduces the number of unknowns to three, as obtained for simple, one-dimensional problems. Basically, the ADIP solves the equations in one direction, with the dependent variable in the second dimension assumed constant over the time interval. As an example, consider equation (11) for the first time step, in the ϕ direction.[5]

$$BT'_{i-1,j} + CT'_{i,j} + DT'_{i+1,j} = Q_{i,j} - AT_{i,j-1} - ET_{i,j+1} \quad (12)$$

---

[4]The SIP boundary condition restrictions are illustrated in the appendix.

[5]Although not specifically pointed out, each time step is split into two parts. The first one-half time step is differenced implicitly in ϕ and explicitly in r, whereas the second one-half time step is differenced implicitly in r and explicitly in ϕ.

The temperatures $T_{i,j-1}$ and $T_{i,j+1}$ are known from the previous time step. Application of equation (12) to a grid network yields a tridiagonal matrix of unknown temperatures. The advantages of solving a tridiagonal matrix rather than a pentadiagonal matrix as generated by equation (11) are evident.

In addition to the previous two methods, the weighted average approach of Crank and Nicolson (ref. 11) was used in conjunction with the SIP algorithm. The Crank-Nicolson (CN) modification is illustrated in the following application to equation (9).

$$
\begin{aligned}
\rho C_p \left(\frac{T'_{i,j} - T_{i,j}}{\Delta t}\right) = \theta \Bigg\{ & k_{i,j}\left[\frac{T'_{i,j+1} - 2T'_{i,j} + T'_{i,j-1}}{(\Delta r)^2}\right] \\
& + \frac{2k_{i,j}}{r_{i,j}}\left(\frac{T'_{i,j+1} - T'_{i,j-1}}{2\ \Delta r}\right) \\
& + \frac{k_{i,j}}{r_{i,j}^2}\left[\frac{T'_{i+1,j} - 2T'_{i,j} + T'_{i-1,j}}{(\Delta\phi)^2}\right] \\
& + \frac{k_{i,j}\cos\phi_{i,j}}{r_{i,j}^2 \sin\phi_{i,j}}\left(\frac{T'_{i+1,j} - T'_{i-1,j}}{2\ \Delta\phi}\right)\Bigg\} \\
& + (1-\theta)\Bigg\{ k_{i,j}\left[\frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{(\Delta r)^2}\right] \\
& + \frac{2k_{i,j}}{r_{i,j}}\left(\frac{T_{i,j+1} - T_{i,j-1}}{2\ \Delta r}\right) \\
& + \frac{k_{i,j}}{r_{i,j}^2}\left[\frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{(\Delta\phi)^2}\right] \\
& + \frac{k_{i,j}\cos\phi_{i,j}}{r_{i,j}^2 \sin\phi_{i,j}}\left(\frac{T_{i+1,j} - T_{i-1,j}}{2\ \Delta\phi}\right)\Bigg\} \\
& + q''' \qquad (13)
\end{aligned}
$$

Equation (13) can be rewritten into the form of equation (11), which is consistent with the SIP formulation. For the CN method, θ is set equal to 0.5 in equation (13).[6] This method is designated simply as SIP/CN.

Because the SIP is an algorithm for solving a certain type of matrix, a table of geometrically arranged iteration parameters is normally employed to speed convergence. Weinstein et al. (ref. 3) recommended a geometrical iteration parameter defined by the relation

$$1 - \gamma_m = \left(1 - \gamma_{max.}\right)^{\frac{m}{n-1}}, \quad m = 0, 1, \ldots (n - 1) \tag{14}$$

where γ is the iteration parameter and n is the number of parameters (normally 4 to 10) in a cycle. The value of the iteration parameter lies between 0 and 1. For a heat-conduction problem with constant properties (ref. 2),

$$\gamma_{max.} = 1 - \min.\left[\frac{2(\Delta r)^2}{1 + \dfrac{k_\phi(\Delta r)^2}{k_r(r\ \Delta\phi)^2}}, \frac{2(r\ \Delta\phi)^2}{1 + \dfrac{k_r(r\ \Delta\phi)^2}{k_\phi(\Delta r)^2}}\right] \tag{15}$$

For this study, a maximum γ value of 0.95 was used. A discussion of the physical and mathematical significances of the iteration parameter can be found in references 2 and 3.

COMPARATIVE NUMERICAL RESULTS

To study the effect of various boundary conditions on the relative accuracy of the solution techniques, the following three examples are considered.[7]

---

[6] Steen and Ali (ref. 5) used weighting values of 0.5 and 0.75.

[7] Any consistent set of units can be used in these examples. In this study, absolute numerical values are used instead of dimensionless quantities, for comparison purposes. Numerical values of $k = 0.8$, $C_p = 0.4$, $\rho = 130$, and $R = 1$ have been used in these examples.

Case 1 - A homogeneous, two-dimensional, uniform surface temperature is specified. The boundary and initial conditions are

$$T(R, \phi, t) = \text{constant surface temperature}$$

$$\frac{\partial T}{\partial r}(0, \phi, t) = 0$$

$$\frac{\partial T}{\partial \phi}(r, \phi, t) = 0, \quad \phi = 0, \pi$$

$$q''' = 0$$

$$T(r, \phi, 0) = T_i$$

This first example is for a sphere with a specified surface temperature. The surface boundary condition is such that $T(R, \phi)$ = constant. An analytic solution is available (ref. 12).

Case 2 - A homogeneous, two-demension, uniform heat generation is specified.

$$T(R, \phi, t) = T(r, \phi, 0))$$
$$= T_i$$

$$\frac{\partial T}{\partial r}(0, \phi, t) = 0$$

$$\frac{\partial T}{\partial \phi}(r, \phi, t) = 0, \quad \phi = 0, \pi$$

$$q'''(r, \phi, t) = \text{constant}$$

Example 2 considers a sphere with uniform internal heat generation. Both the initial and surface temperatures are set equal to zero. An analytic solution for this case can be found in reference 13.

Case 3 - A homogeneous, two-dimensional, nonuniform surface temperature is specified.

$$T(R, \phi, t) = R^2 \left(\frac{3 \cos 2\phi + 1}{4}\right)$$

$$\frac{\partial T}{\partial r}(0, \phi, t) = 0$$

$$\frac{\partial T}{\partial \phi}(r, \phi, t) = 0, \quad \phi = 0, \pi$$

$$q''' = 0$$

$$T(r, \phi, 0) = 0$$

This third example considers a sphere of unit radius $R = 1$, with the surface temperature specified as a function of $\cos \phi$. An analytic solution for this case is presented in reference 7.

It should be noted that cases 1 and 2 are one-dimensional problems; however, the numerical computations were performed with the use of a two-dimensional model. Case 3 is used to represent the accuracy of the numerical techniques for a two-dimensional problem with a zero temperature along $\phi = 54.7356$ degrees and $\phi = 125.2644$ degrees for all values of r. For these cases, the results are given in terms of the difference between the temperature obtained by the exact solution and that obtained form the various numerical solution techniques. These results are called the temperature errors, defined as $T_{exact} - T_{cal.}$. As a convenient reference for comparing the numerical data, table I summarizes the various conditions used to generate the results given in tables II through IV. For example, numerical time-step effects can be studied by reference to tables II(a) and II(b). Tables II(a) through II(c) present a comparison of the numerical results for locations within a sphere with a specified constant surface temperature condition of $r/R = 0$ and $r/R = 0.5$. The temperature history at the geometrical center, $r/R = 0$, is of special interest because a discontinuity in equation (3) occurs at this location. A comparison of the results at $r = 0$ indicates that the SIP with CN modification (SIP/CN) with a geometrically variable γ and the ADIP are the most accurate. A maximum temperature error of 30.631 degrees (3.96 percent error) occurred at a time unit of 10 after the start of the transient. Although no ϕ variation in the surface temperature was specified, where a ϕ variation in the temperature was calculated, the error range in the ϕ direction is shown.

The standard SIP methods (constant and variable γ) had the greatest absolute errors. Also shown in tables II(a) through II(c) are the hollow-sphere and rectangular approximation solutions used at $r = 0$. Again, a large absolute error was found for these two approximate solutions. The effect of the time step is shown in tables II(a) through II(c): reduction of the time step to $\Delta t = 0.1$ resulted in a significant reduction in the absolute error for all methods investigated. The effect of location, $r/R = 0.5$, on error again shows the SIP/CN (variable γ) and ADIP methods to be the most accurate.

The effect of node size on accuracy can be seen by comparing the results of tables II(b) and II(d) for $r = 0$, $\Delta t = 1.0$. For a reduction of $\Delta r = 0.10$ to $\Delta r = 0.05$, the error with use of the SIP (γ = constant) increased from 30.631 to 92.310 degrees for $\Delta t = 1.0$. A similar increase in the temperature error for the SIP/CN (γ = variable) and the ADIP was experienced.[8]

However, for a node reduction of $\Delta r = 0.1$ to $\Delta r = 0.05$, at a time step of $\Delta t = 0.10$, the absolute error decreased for both the SIP/CN and the ADIP methods. The results in tables II(a) through II(e) clearly indicate the effect of time step and node size on numerical accuracy for the SIP approach.

Tables III(a) and III(b) present the numerical results for a sphere with internal heat generation. Once again, the SIP/CN (variable γ) and the ADIP methods are the most accurate. For this particular case, a reduction in the time step of $\Delta t = 1.0$ to $\Delta t = 0.1$ resulted in a greater accuracy, in general, for the five methods, except for the SIP/CN (variable γ) and the ADIP methods.

Tables IV(a) through IV(g) present the numerical results for a sphere with the surface temperature specified as a $\cos \phi$ function. Table IV(a) is the analytic solution as outlined in reference 7. For case 3, both an absolute error defined by

$$T_{error} = T_{exact} - T_{cal.}$$

and a relative error defined by

$$T_{rel} = \frac{T_{exact} - T_{cal.}}{T_{exact}}$$

were used to evaluate the numerical procedures. Tables IV(b), IV(d), and IV(f) show the steady-state absolute error for ADIP, SIP/CN (α = variable), and SIP (α = variable)/hollow-sphere approximation, respectively. Tables IV(c), IV(e), and IV(g) show the relative error for the respective methods. As expected, the least error occurs for r values near $R = 1$ and for ϕ values greater than 55 degrees and 125 degrees. As r approaches zero, the relative error increases quite rapidly. This same effect is observed as ϕ approaches 55.74 degrees and 125.26 degrees, where temperature is zero for r values. These errors are a result of the assumption (e.g., eq. 5) used in numerical procedures and illustrate the sensitivity when the solution is zero. Similar results are shown by Kee in reference 7, where the restrictions of equations (8a) and (8b) were not employed.

[8] A similar result was also noted by Barakat and Clark (ref. 14).

CONCLUDING REMARKS

Two basic numerical solutions (the strongly implicit procedure (SIP) and the alternating-direction implicit procedure (ADIP)) to the diffusion equation in spherical coordinates have been presented. The validity and accuracy of these solutions are demonstrated by comparing the results obtained therby with those of analytical solutions. Previous studies have shown that both methods compare favorably for the diffusion equation in Cartesian coordinates. The standard SIP appears to be slightly less efficient than the ADIP for the solid spherical problem studied in this investigation. This decrease in efficiency may be a direct result of the requirement that the dependent variable be calculated for the center of the sphere, where a discontinuity in the governing equation occurs. However, the Crank-Nicolson modification of the SIP gave essentially the same results as the ADIP for the cases studied.

In conclusion, it should be mentioned that the SIP algorithm has been shown to be far superior to the ADIP for simulation problems involving multiphase flow in porous media. It has been possible to obtain converged solutions to coupled systems of partial differential equations with the SIP when both the ADIP and successive over-relaxation procedures have failed. It should also be pointed out that a comparison in which a constant-property rectangular region was used showed the ADIP to be superior to the SIP, but the SIP was shown more efficient for other rectangular cases involving property anisotrophy and/or irregular boundary conditions.

Lyndon B. Johnson Space Center
National Aeronautics and Space Administration
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TABLE I.- SUMMARY OF CONDITIONS STUDIED

r/R	Δt	Δr	Table no.	Remarks
Case 1				
0	0.1	0.10	II(a)	
0	1.0	.10	II(b)	
.5	1.0	.10	II(c)	
0	1.0	.05	II(d)	
0	.1	.05	II(e)	
Case 2				
0.5	1.0	0.10	III(a)	
.5	.1	.10	III(b)	
Case 3				
--	--	--	IV(a)	Analytical solution
--	1.0	0.025	IV(b), IV(c)	ADIP
--	1.0	.025	IV(d), IV(e)	SIP/CN (α = variable)
--	1.0	.025	IV(f), IV(g)	SIP (α = variable)/ hollow-sphere approximation

TABLE II.- CASE 1

(a) $r/R = 0$; $\Delta t = 0.1$; $\Delta r = 0.10$

Method	Temperature error $(T_{exact} - T_{cal.})^a$, deg, at a time unit and corresponding T_{exact} of -			
	5	10	20	50
	597.833°	773.586°	918.735°	959.566°
SIP ($\gamma = \gamma_{max.}$)	-3.672 -3.756	2.606 2.533	1.815 1.797	0.054
SIP (γ = variable)	-4.074	2.146	1.637	.049
SIP/CN ($\gamma = \gamma_{max.}$)	-2.978 -3.006	.563 .540	.735 .731	.025
SIP/CN (γ = variable)	-3.099	.428	.685	.023
ADIP	-3.037	.425	.680	.026
SIP ($\gamma = \gamma_{max.}$)/ hollow-sphere approximation	2.973	7.805	1.969	-1.384
SIP ($\gamma = \gamma_{max.}$)/ rectangular approximation	3.862	9.017	3.355	.071

[a] T_{exact} = exact temperature; $T_{cal.}$ = calculated temperature.

TABLE II.- Continued

(b) $r/R = 0$; $\Delta t = 1.0$; $\Delta r = 0.10$

Method	Temperature error $(T_{exact} - T_{cal.})^a$, deg, at a time unit and corresponding T_{exact} of -			
	5 597.833°	10 773.586°	20 918.735°	50 959.566°
SIP ($\gamma = \gamma_{max.}$)	-3.094 -.198	30.631 25.886	17.254 15.798	0.572 .547
SIP (γ = variable)	-10.293	15.585 15.485	10.309 10.283	.334
SIP/CN ($\gamma = \gamma_{max.}$)	.141 4.255	9.986 4.886	3.914 2.959	.09 .07
SIP/CN (γ = variable)	-.821	.304	.460 .455	.017
ADIP	1.095	-1.13	-.306	-.002
SIP ($\gamma = \gamma_{max.}$)/ hollow-sphere approximation	8.019	35.133	17.083	-.875
SIP ($\gamma = \gamma_{max.}$)/ rectangular approximation	8.525	36.094	18.456	-.145

[a] T_{exact} = exact temperature; $T_{cal.}$ = calculated temperature.

TABLE II.- Continued

(c) $r/R = 0.5$; $\Delta t = 1.0$; $\Delta r = 0.10$

Method	Temperature error $(T_{exact} - T_{cal.})^a$, deg, at a time unit and corresponding T_{exact} of -			
	5	10	20	50
	703.751°	840.065°	933.727°	959.724°
SIP ($\gamma = \gamma_{max.}$)	15.247 15.472	18.891 18.816	9.563 9.486	0.339 .338
SIP (γ = variable)	10.301	13.576	6.583 6.580	.213
SIP/CN ($\gamma = \gamma_{max.}$)	1.150 1.114	2.189 2.162	1.298 1.259	.041
SIP/CN (γ = variable)	-.880	.165	.289	.011
ADIP	3.118	-.867	-.285	-.002
SIP ($\gamma = \gamma_{max.}$)/ hollow-sphere approximation	15.247 14.288	18.891 18.309	9.563 9.364	.338
SIP ($\gamma = \gamma_{max.}$)/ rectangular approximation	15.247 14.288	18.891 18.816	9.563 9.364	.338

[a] T_{exact} = exact temperature; $T_{cal.}$ = calculated temperature.

TABLE II.- Continued

(d) $r/R = 0$; $\Delta t = 1.0$; $\Delta r = 0.05$

Method	Temperature error $(T_{exact} - T_{cal.})^{a}$, deg, at a time unit and corresponding T_{exact} -			
	5	10	20	50
	597.833°	773.586°	918.735°	959.566°
SIP ($\gamma = \gamma_{max.}$)	28.523 33.555	92.310 80.253	55.256 50.143	2.751 2.579
SIP (γ = variable)	2.065 4.606	32.138 28.219	16.972 15.838	.536 .517
SIP/CN ($\gamma = \gamma_{max.}$)	18.454 30.451	54.256 26.880	25.711 16.714	1.251 .924
SIP/CN (γ = variable)	2.568 6.652	10.233 1.126	5.869 1.013	.203 .288
ADIP	3.640	-1.951	-.889	-.013

[a]T_{exact} = exact temperature; $T_{cal.}$ = calculated temperature.

TABLE II.- Concluded

(e) $r/R = 0$; $\Delta t = 0.1$; $\Delta r = 0.05$

Method	Temperature error $(T_{exact} - T_{cal.})$[a], deg, at a time unit and corresponding T_{exact} of -			
	5	10	20	50
	597.833°	773.586°	918.735°	959.566°
SIP ($\gamma = \gamma_{max.}$)	1.460 1.572	6.112 6.206	2.884 2.900	0.073
SIP (γ = variable)	-1.799 -1.798	1.888 1.887	1.123 1.124	.028
SIP/CN ($\gamma = \gamma_{max.}$)	.152 .417	1.384 1.583	.723 .756	.017
SIP/CN (γ = variable)	-.768	.112	.168	.003
ADIP	-.699	.110	.166	.008

[a] T_{exact} = exact temperature; $T_{cal.}$ = calculated temperature.

TABLE III.- CASE 2

(a) $r/R = 0.5$; $\Delta t = 1.0$; $\Delta r = 0.10$

Method	Temperature error $(T_{exact} - T_{cal.})^a$, deg, at a time unit and corresponding T_{exact} of -		
	10 2.41849°	30 3.0911°	50 3.12337°
SIP ($\gamma = \gamma_{max.}$)	0.12552 .12407	0.02150 .02117	0.00206 .00203
SIP (γ = variable)	.08681 .08676	.01411	.00127
SIP/CN ($\gamma = \gamma_{max.}$)	.02132 .02030	.00319 .00317	.00026
SIP/CN (γ = variable)	.00679	.00099	.00008
ADIP	.00038	.00010	0

[a] T_{exact} = exact temperature; $T_{cal.}$ = calculated temperature.

TABLE III.- Concluded

(b) $r/R = 0.5$; $\Delta t = 0.1$; $\Delta r = 0.10$

Method	Temperature error $(T_{exact} - T_{cal.})^a$, deg, at a time unit and corresponding T_{exact} of -		
	10 2.41849°	30 3.0911°	50 3.12337°
SIP ($\gamma = \gamma_{max.}$)	0.01796 .01788	0.00266	0.00021
SIP (γ = variable)	.01689	.00250	.00020
SIP/CN ($\gamma = \gamma_{max.}$)	.00910 .00908	.00134	.00011
SIP/CN (γ = variable)	.0088	.00129	.00010
ADIP	.00874	.00129	.00011

[a] T_{exact} = exact temperature; $T_{cal.}$ = calculated temperature.

TABLE IV.- CASE 3

(a) Analytic solution

Angular position (ϕ), deg	Temperature (T), deg, at a radial position (r) of -						
	1.00	0.75	0.50	0.25	0.15	0.10	0.05
0	1.0000	0.56250	0.250000	0.062500	0.02250	0.01000	0.002500
18.46150	.849582	.477890	.212395	.0530989	.0191156	.00849582	.00212396
36.9231	.458663	.257998	.114666	.0286664	.0103199	.00458663	.00114666
55.3846	-.0159537	-.00897393	-.00398841	-.000997103	-.000358957	-.000159537	-.0000398841
73.8462	-.383892	-.215940	-.0959731	-.0239933	-.00863758	-.00383893	-.000959731
83.0769	-.478206	-.268991	-.119552	-.0298879	-.0107596	-.00478206	-.00119552
96.9231	-.478206	-.268991	-.119552	-.0298879	-.0107596	-.00478206	-.00119552
106.1540	-.383893	-.215940	-.0959731	-.0239933	-.00863758	-.00383893	-.000959732
124.615	-.0159538	-.00897404	-.00398846	-.000997115	-.000358961	-.000159538	-.0000398846
143.077	.458663	.257998	.114666	.0286664	.0103199	.00458663	.00114666
161.538	.849582	.477890	.212395	.0530989	.0191156	.00849582	.00212395
180.00	1.0000	.56250	.250000	.062500	.02250	.01000	.002500

TABLE IV.- Continued

(b) ADIP - absolute error at steady-state

Angular position (ϕ), deg	Temperature absolute error $(T_{exact} - T_{cal.})^a$, deg, at a radial position (r) of -						
	1.00	0.75	0.50	0.25	0.15	0.10	0.050
0	0	-0.000708	-0.000864	-0.0006358	-0.0004991	-0.0004358	-0.00038490
18.46150	0	-.000632	-.000779	-.0005919	-.0004773	-.00042402	-.00038105
36.9231	0	-.000414	-.000544	-.0004749	-.0004196	-.00039289	-.00037093
55.3846	0	-.00014885	-.00026036	-.000332609	-.000349454	-.00035506	-.000358630
73.8462	0	.000057	-.0000398	-.0002223	-.00029508	-.00032572	-.000349093
83.0769	0	.00011	.000016	-.000194	-.0002811	-.0003182	-.000346652
96.9231	0	.00011	.000016	-.000194	-.0002811	-.0003182	-.000346652
106.1540	0	.000057	-.0000398	-.0002223	-.00029507	-.00032573	-.000349094
124.6150	0	-.0001488	-.00026034	-.000332612	-.000349456	-.00035507	-.000358633
143.077	0	-.000414	-.000544	-.0004749	-.0004196	-.00039290	-.00037093
161.538	0	-.000632	-.000779	-.0005919	-.0004773	-.00042403	-.00038107
180.00	0	-.000708	-.000864	-.0006359	-.0004991	-.0004358	-.00038491

[a] T_{exact} = exact temperature; T_{cal} = calculated temperature.

TABLE IV.- Continued

(c) ADIP - relative error at steady-state

Angular position (ϕ), deg	Temperature relative error $((T_{exact} - T_{cal.})/T_{exact})$[a] at a radial position (r) of -						
	1.00	0.75	0.50	0.25	0.15	0.10	0.050
0	0	-0.0012587	-0.003456	-0.010173	-0.022182	-0.043580	-0.15396
18.46150	0	-.0013225	-.003667	-.011147	-.024969	-.049910	-.179410
36.9231	0	-.0016047	-.0047445	-.016568	-.040659	-.085660	-.32349
55.3846	0	.016587	.065279	.33358	.97353	2.2256	8.9918
73.8462	0	-.00026396	.00041470	.0092651	.034162	.084847	.36374
83.0769	0	-.00040894	-.00013383	.0064909	.026126	.066540	.28996
96.9231	0	-.00040894	-.00013383	.0064909	.026126	.066540	.28996
106.1540	0	-.00026396	.00041470	.0092651	.034161	.084847	.36374
124.6150	0	.016581	.065273	.33357	.97352	2.2256	8.9918
143.077	0	-.0016047	-.0047445	-.016568	-.040659	-.085662	-.32349
161.538	0	-.0013225	-.0036677	-.011147	-.024969	-.049910	-.17942
180.00	0	-.0012587	-.003456	-.010174	-.022182	-.043580	-.15396

[a] T_{exact} = exact temperature; $T_{cal.}$ = calculated temperature.

TABLE IV.- Continued

(d) SIP/CN (α = variable) - absolute error at steady-state

Angular position (ϕ), deg	Temperature absolute error ($T_{exact} - T_{cal.}$)[a], deg, at a radial position (r) of -						
	1.00	0.75	0.50	0.25	0.15	0.10	0.050
0	0	-0.000716	-0.000865	-0.0006096	-0.0004465	-0.0003796	-0.00033054
18.46150	0	-.000640	-.000779	-.0005912	-.0004793	-.00042905	-.00036815
36.9231	0	-.000418	-.000544	-.0004747	-.0004187	-.00039283	-.00037706
55.3846	0	-.00014826	-.00026011	-.000332297	-.000349282	-.000353759	-.00036516
73.8462	0	.00006	-.0000395	-.000222	-.00029488	-.00032509	-.000351408
83.0769	0	.000115	.000017	-.0001937	-.0002808	-.00031788	-.0003467
96.9231	0	.000115	.000017	-.0001937	-.0002808	-.00031826	-.000343674
106.1540	0	.00006	-.0000395	-.000222	-.00029472	-.0003260	-.00034447
124.615	0	-.00014832	-.0002602	-.000332423	-.000349284	-.00035566	-.0003517636
143.077	0	-.000418	-.000544	-.0004747	-.0004198	-.00039245	-.0003648
161.538	0	-.000639	-.000779	-.0005922	-.0004752	-.00041672	-.00039205
180.00	0	-.000716	-.000865	-.0006958	-.0006199	-.0005674	-.00051088

[a] T_{exact} = exact temperature; $T_{cal.}$ = calculated temperature.

TABLE IV.- Continued

(e) SIP/CN (α = variable) - relative error at steady-state

Angular position (ϕ), deg	Temperature relative error $((T_{exact} - T_{cal.})/T_{exact})^{a}$ at a radial position (r) of -						
	1.00	0.75	0.50	0.25	0.15	0.10	0.050
0	0	-0.0012729	-0.00346	-0.0097536	-0.019844	-0.03796	-0.132216
18.46150	0	-.0013392	-.0036677	-.011134	-.025074	-.05050	-.17333
36.9231	0	-.0016202	-.0047442	-.016559	-.040572	-.085647	-.32883
55.3846	0	.016521	.065216	.33326	.97305	2.2174	9.15553
73.8462	0	-.00027785	-.00041157	.0092526	.034139	.084682	.36615
83.0769	0	.00042752	-.0001422	.0064809	.026098	.066473	.28999
96.9231	0	.00042752	-.0001422	.0064809	.026098	.066552	.28747
106.1540	0	-.00027785	-.00041157	.0092526	.034121	.084919	.35892
124.615	0	.016528	.065236	.33338	.97304	2.2293	8.81953
143.077	0	-.0016202	-.0047442	-.016559	-.040679	-.085564	-.31814
161.538	0	-.0013371	-.0036677	-.011153	-.024859	-.049050	-.18459
180.00	0	-.0012729	-.00346	-.011133	-.027551	-.05674	-.204352

[a] T_{exact} = exact temperature; $T_{cal.}$ = calculated temperature.

TABLE IV.- Continued

(f) SIP/hollow-sphere approximation (α = variable) - absolute error at steady-state

Angular position (ϕ), deg	Temperature absolute error ($T_{exact} - T_{cal.}$)[a], deg, at a radial position (r) of -						
	1.00	0.75	0.50	0.25	0.15	0.10	0.050
0	0	-0.000706	-0.000862	-0.0006318	-0.0004942	-0.0004307	-0.00037945
18.46150	0	-.000631	-.000777	-.0005878	-.0004724	-.0004186	-.00037561
36.9231	0	-.000413	-.000542	-.0004707	-.0004147	-.00038774	-.00036554
55.3846	0	-.00014737	-.00025767	-.00032823	-.000344577	-.000349924	-.0003532921
73.8462	0	.000058	-.0000369	-.0002179	-.00029017	-.0003206	-.000343794
83.0769	0	.000112	-.000019	-.0001896	-.0002762	-.00031307	-.000341364
96.9231	0	.000112	-.000019	-.0001896	-.0002762	-.00031307	-.000341367
106.1540	0	.000058	-.0000369	-.0002179	-.00029017	-.0003206	-.000343803
124.6150	0	-.00014733	-.00025766	-.000328325	-.000344587	-.000349936	-.0003533106
143.077	0	-.000413	-.000542	-.0004707	-.0004148	-.00038777	-.00036557
161.538	0	-.000631	-.000777	-.0005878	-.0004725	-.0004189	-.00037567
180.00	0	-.000706	-.000862	-.0006318	-.0004943	-.0004307	-.0003795

[a] T_{exact} = exact temperature; $T_{cal.}$ = calculated temperature.

TABLE IV.- Concluded

(g) SIP/hollow-sphere approximation (α = variable) - relative error at steady-state

Angular position (ϕ), deg	Temperature relative error $((T_{exact} - T_{cal.})/T_{exact})$[a] at a radial position (r) of -						
	1.00	0.75	0.50	0.25	0.15	0.10	0.050
0	0	-0.0012551	-0.003448	-0.010109	-0.021964	-0.04307	-0.15178
18.6415	0	-.0013204	-.0036583	-.011070	-.024713	-.049302	-.17684
36.9231	0	-.0016008	-.0047268	-.016420	-.040184	-.084537	-.31879
55.3846	0	.016422	.064605	.32918	.95994	2.1934	8.8580
73.8462	0	-.00026859	.00038448	.0090817	.039594	.083513	.35822
83.0769	0	-.00041637	.00015893	.0063437	.025670	.065468	.28554
96.9231	0	-.00041637	.00015893	.0063437	.025670	.065468	.28554
106.1540	0	-.00026859	.00038448	.0090817	.033594	.083513	.35823
124.6150	0	.016417	.064601	.32927	.95996	2.1934	8.8583
143.077	0	-.0016008	-.0047268	-.016420	-.040194	-.084544	-.31881
161.538	0	-.0013204	-.0036583	-.011070	-.024718	-.049302	-.17687
180.00	0	-.0012551	-.003448	-.010109	-.021969	-.04307	-.15178

[a] T_{exact} = exact temperature; $T_{cal.}$ = calculated temperature.

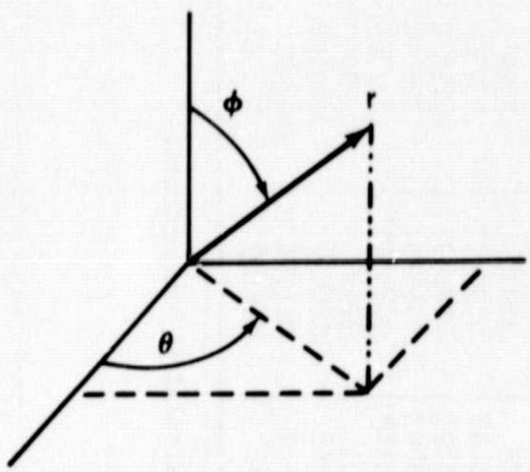

Figure 1.- Spherical coordinate system.

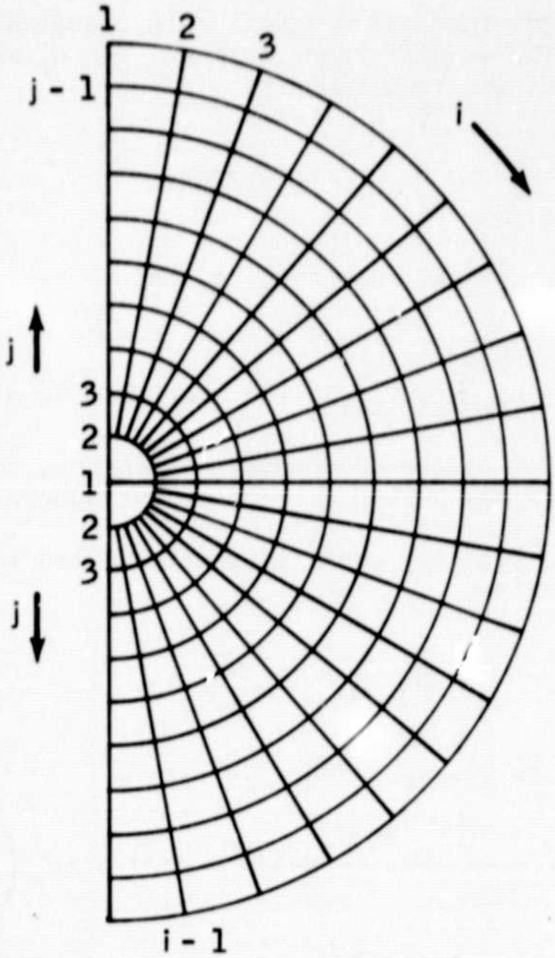

Figure 2.- Finite-difference grid network.

APPENDIX

BOUNDARY CONDITION RELATIONS WITH USE OF THE STRONGLY IMPLICIT TECHNIQUE

The transient-heat-conduction equation in spherical coordinates (eq. (3)) is put in finite-difference form at $r = 0$ as an illustration of the SIP boundary condition requirements.

SOLID SPHERE

The SIP boundary restrictions require that

$$A_{i,o};\ E_{i,R} = 0 \quad \text{for} \quad \phi = 0,\ \pi \tag{16}$$

$$B_{\phi=0,j};\ D_{\phi=\pi,j} = 0 \quad \text{for} \quad r = 0,\ R \tag{17}$$

As an illustration of these boundary conditions, consider the singularity located at the geometrical center, $r = 0$, of the sphere.

By employing the boundary conditions represented by equations (8a) and (8b), equation (3) becomes

$$\rho C_p \frac{\partial T}{\partial t} = 3k \frac{\partial^2 T}{\partial r^2} + q''' \tag{18}$$

which can be written in finite-difference form as

$$\frac{k_{i,j}\left(3T'_{i,j+1} - 6T'_{i,j} + 3T'_{i,j-1}\right)}{(\Delta r)^2} + q''' = \rho C_p \left(\frac{T'_{i,j} - T_{i,j}}{\Delta t}\right) \tag{19}$$

Employing equation (5) yields

$$T_{i,j+1} = T_{i,j-1} \tag{20}$$

Then, equation (19) can be written as

$$-\left[\frac{6k_{i,j}}{(\Delta r)^2} + \frac{\rho C_p}{\Delta t}\right] T'_{i,j} + \frac{6k_{i,j}}{(\Delta r)^2} T'_{i,j+1} = -q''' - \frac{\rho C_p}{\Delta t} T_{i,j} \tag{21}$$

Comparing equation (21) with equation (11) yields

$$C_{i,j}T'_{i,j} + E_{i,j}T'_{i,j+1} = Q_{i,j} \tag{22}$$

where

$$A_{0,j} \equiv B_{0,j}$$

$$\equiv D_{0,j}$$

$$= 0 \tag{23a}$$

and

$$C_{0,j} = -\left[\frac{6k_{0,j}}{(\Delta r)^2} + \frac{\rho C_p}{\Delta t}\right] \tag{23b}$$

$$E_{0,j} = \frac{6k_{0,j}}{(\Delta r)^2} \tag{23c}$$

$$Q_{0,j} = -\frac{\rho C_p}{\Delta t} T_{i,j} - q'''_{0,j} \tag{23d}$$

HOLLOW-SPHERE APPROXIMATION

This approximation assumes that a small but finite radius (r_o) can be used to represent the geometrical center. To illustrate this boundary condition, consider the location

$$r = r_o\left(r_o = 0.01\ \Delta r\right), \quad \phi = 0$$

By employing the boundary conditions represented by equation (8c) and

$$\left.\frac{\partial T}{\partial r}\right|_{r=r_o} = 0$$

equation (3) becomes

$$k\frac{\partial^2 T}{\partial r^2} + \frac{2k}{r_o}\frac{\partial^2 T}{\partial \phi^2} + q''' = \rho C_p \frac{\partial T}{\partial t} \tag{24}$$

With the assumptions that at

$$\phi = 0, \quad T'_{i-1,j} = T'_{i+1,j} \tag{25a}$$

$$r = r_o, \quad T'_{i,j-1} = T'_{i,j+1} \tag{25b}$$

equation (24) can be formulated in terms of equation (11) as

$$C_{0,r_o} T'_{i,j} + D_{0,r_o} T'_{i+1,j} + E_{0,r_o} T'_{i,j+1} = Q_{0,r_o} \tag{26}$$

where

$$C_{0,r_o} = -\left[\frac{2k_{0,r_o}}{(\Delta r)^2} + \frac{4k_{0,r_o}}{\left(r_o\ \Delta\phi\right)^2} + \frac{\rho C_p}{\Delta t}\right] \tag{27a}$$

$$D_{0,r_o} = \frac{4k_{0,r_o}}{\left(r_o\ \Delta\phi\right)^2} \tag{27b}$$

$$E_{0,r_o} = \frac{2k_{0,r_o}}{(\Delta r)^2} \tag{27c}$$

$$Q_{0,r_o} = -\frac{\rho C_p}{\Delta t} T_{0,r_o} - q'''_{0,r_o} \tag{27d}$$