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Numerical Solution of the 3-Dimensional Heat Flow Equation

ABSTRACT

A numerical differencing scheme is outlined that gives the investigator a fast, accurate research tool. The scheme uses an extrapolation routine coupled with a line solution technique to solve the heat flow equation. The technique applies equally well to line or plane symmetry: 2-dimensional as well as fully 3-dimensional problems.

Heat flow problems are commonly handled in an analytical fashion, e.g., as in Carslaw and Jaeger (1959) and Ingersoll, *et al.* (1954). However, many problems in heat flow cannot be handled in a classical fashion and various finite difference techniques must be used. Explicit, successive over relaxation and alternating direction implicit (ADI) techniques are commonly employed differencing schemes used in the solution of heat or fluid flow problems (e.g., see Smith, 1965; Zienkiewicz, 1967; Carnahan, *et al.*, 1969; Von Rosenberg, 1969). Depending upon the problem, various differencing forms are superior to others in terms of computer time, accuracy, or general ease of programming.

The primary purpose of this investigation was to develop a differencing scheme that is fast, has a high order of accuracy, and is simple to iterate provided that the non-linear form of the heat flow equation is the solution objective.

The differential equation of heat flow can be expressed as

$$\frac{\partial}{\partial x}\left(\kappa \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\kappa \frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(\kappa \frac{\partial T}{\partial z}\right) + Q = Cp\,\rho\,\frac{\partial T}{\partial t} \qquad (1)$$

where

- T = temperature (°F)
- t = time T
- Q = heat generation rate per unit volume Btu/L^3-T
- Cp = specific heat Btu/lb-°F
- ρ = density lb/L^3
- κ = thermal conductivity Btu/T-L-°F

The Crank-Nicholson differencing scheme is used to approximate (1). This scheme is unconditionally stable and has an error of

$$e = O(\Delta x^2) + O(\Delta y^2) + O(\Delta z^2) + O(\Delta t^2).$$

The resulting system of linear equations forms a tri-diagonal matrix that is solved using the Thomas algorithm (see, for example, Von Rosenberg, 1969). The linear equations require two unknown values of temperature at the n+1 time step, the unknown values of temperature are extrapolated and the equations solved for the n+1 time. The extrapolation routine used is

$$T^{n+2}_{i,j,k} = T^{n+1}_{i,j,k} + \frac{\Delta t^{n+\frac{1}{2}}}{\Delta t^{n-\frac{1}{2}}}\left(T^{n+1}_{i,j,k} - T^{n}_{i,j,k}\right)$$

The computed value of temperature is compared to the extrapolated value and if the differences are greater than some epsilon, the computed value replaces the extrapolated value and the computer solves the linear equations again. This iterate term is compared again and the iterations continue until the difference between two successive iterates is below epsilon.

The difference equation is:

$$\begin{aligned}
&\frac{1}{\Delta x_i}\left[K_{i+\frac{1}{2}}\frac{\left(T^{n+\frac{1}{2}}_{i+1,j,k} - T^{n+\frac{1}{2}}_{i,j,k}\right)}{\Delta x_{i+\frac{1}{2}}} - K_{i-\frac{1}{2}}\frac{\left(T^{n+\frac{1}{2}}_{i,j,k} - T^{n+\frac{1}{2}}_{i-1,j,k}\right)}{\Delta x_{i-\frac{1}{2}}}\right] + \\
&\frac{1}{\Delta y_i}\left[K_{j+\frac{1}{2}}\frac{\left(T^{n+\frac{1}{2}}_{i,j+1,k} - T^{n+\frac{1}{2}}_{i,j,k}\right)}{\Delta y_{j+\frac{1}{2}}} - K_{j-\frac{1}{2}}\frac{\left(T^{n+\frac{1}{2}}_{i,j,k} - T^{n+\frac{1}{2}}_{i,j-1,k}\right)}{\Delta y_{j-\frac{1}{2}}}\right] + \\
&\frac{1}{\Delta z_k}\left[K_{k+\frac{1}{2}}\frac{\left(T^{n+\frac{1}{2}}_{i,j,k+1} - T^{n+\frac{1}{2}}_{i,j,k}\right)}{\Delta z_{k+\frac{1}{2}}} - K_{k-\frac{1}{2}}\frac{\left(T^{n+\frac{1}{2}}_{i,j,k} - T^{n+\frac{1}{2}}_{i,j,k-1}\right)}{\Delta z_{k-\frac{1}{2}}}\right] = \\
&\frac{\left(T^{n+1}_{i,j,k} - T^{n}_{i,j,k}\right)}{\Delta t^{n+\frac{1}{2}}}\left(Cp\,\rho\right)_{i,j,k}
\end{aligned} \qquad (2)$$

and K_i, K_j, K_k are $\kappa_{x(i,j,k)}$, $\kappa_{y(i,j,k)}$, and $\kappa_{z(i,j,k)}$ respectively; and κ_x, κ_y, κ_z are the thermal conductivities for the x, y, and z directions in node (i,j,k). $(C_p\,\rho)_{i,j,k}$ is the specific heat times the density in node (i,j,k). Defining:

$$T^{n+\frac{1}{2}}_{i,j,k} = \tfrac{1}{2}\left(T^{n+1}_{i,j,k} + T^{n}_{i,j,k}\right) \qquad (3)$$

and assuming (in this development) equal spacing in each layer ($\Delta x = \Delta y$) and constant spacing in all

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directions, then:

$$\Delta x_i = \Delta x_{i+1}$$
$$\Delta y_j = \Delta y_{j+1}$$
$$\Delta z_k = \Delta z_{k+1}$$

$$\frac{1}{\Delta x_i \Delta x_{i+\frac{1}{2}}} = \frac{1}{\Delta x^2} = \frac{1}{\Delta y^2} = \frac{1}{\Delta z^2} \quad (4)$$

and similar equations can be developed for spacing, $i-\frac{1}{2}$, $j+\frac{1}{2}$, $j-\frac{1}{2}$, $k-\frac{1}{2}$, $k+\frac{1}{2}$. We also can define:

$$K_{i+\frac{1}{2}} = \frac{2\ K_{i+1}\ K_i}{K_{i+1} + K_i} \quad (5)$$

and here also similar equations can be developed for conductivities at $i-\frac{1}{2}$, $j+\frac{1}{2}$, $j-\frac{1}{2}$, $k+\frac{1}{2}$, $k-\frac{1}{2}$.

For simplicity let

$$A_i = \frac{1}{\Delta x^2} = \frac{1}{\Delta y^2} \quad (6)$$

$$B_k = \frac{1}{\Delta z^2} \quad (7)$$

$$AX_{i+1,j,k} = K_{i+\frac{1}{2}} = \frac{2K_{i+1}\ K_i}{K_{i+1} + K_i} \quad (8)$$

$$BX_{i-1,j,k} = K_{i-\frac{1}{2}} = \frac{2K_{i-1}\ K_i}{K_{i-1} + K_i} \quad (9)$$

$$CX_{i,j+1,k} = K_{j+\frac{1}{2}} = \frac{2K_{j+1}\ K_j}{K_{j+1} + K_j} \quad (10)$$

$$DX_{i,j-1,k} = K_{j-\frac{1}{2}} = \frac{2K_{j-1}\ K_j}{K_{j-1} + K_j} \quad (11)$$

$$EX_{i,j,k+1} = K_{k+\frac{1}{2}} = \frac{2K_{k+1}\ K_k}{K_{k+1} + K_k} \quad (12)$$

$$FX_{i,j,k-1} = K_{k-\frac{1}{2}} = \frac{2K_{k-1}\ K_k}{K_{k-1} + K_k} \quad (13)$$

$$E_{i,j,k} = \frac{2(Cp\ \rho)_{i,j,k}}{\Delta t} \quad (14)$$

$$Q'_{i,j,k} = \frac{2Q_{i,j,k}}{\Delta x^2 \Delta z} \quad (15)$$

Substituting into equation (2), collecting like terms, and simplifying yields:

$$A_i\ AX_{i,j,k}\ (T^{n+1}_{i+1,j,k} - T^{n+1}_{i,j,k}) - A_i\ BX_{i,j,k}\ (T^{n+1}_{i,j,k} - T^{n+1}_{i-1,j,k})$$
$$+ A_i\ CX_{i,j,k}\ (T^{n+1}_{i,j+1,k} - T^{n+1}_{i,j,k}) - A_i\ DX_{i,j,k}\ (T^{n+1}_{i,j,k} - T^{n+1}_{i,j-1,k}) +$$
$$B_k\ EX_{i,j,k}\ (T^{n+1}_{i,j,k+1} - T^{n+1}_{i,j,k}) - B_k\ FX_{i,j,k}\ (T^{n+1}_{i,j,k} - T^{n+1}_{i,j,k-1}) = \quad (16)$$
$$- A_i\ AX_{i,j,k}\ (T^{n}_{i+1,j,k} - T^{n}_{i,j,k}) + A_i\ BX_{i,j,k}\ (T^{n}_{i,j,k} - T^{n}_{i-1,j,k})$$
$$- A_i\ CX_{i,j,k}\ (T^{n}_{i,j+1,k} - T^{n}_{i,j,k}) + A_i\ DX_{i,j,k}\ (T^{n}_{i,j,k} - T^{n}_{i,j-1,k})$$
$$- B_k\ EX_{i,j,k}\ (T^{n}_{i,j,k+1} - T^{n}_{i,j,k}) + B_k\ FX_{i,j,k}\ (T^{n}_{i,j,k} - T^{n}_{i,j,k-1})$$
$$+ E_{i,j,k}\ (T^{n+1}_{i,j,k} - T^{n}_{i,j,k}) - Q'_{i,j,k}$$

Letting $G_{i,j,k}$ equal all the terms on the right-hand side except $E_{i,j,k}$, equation (16) can be rewritten as follows:

$$- T^{n+1}_{i,j,k}\ (A_i\ AX_{i,j,k} + A_i\ BX_{i,j,k} + A_i\ CX_{i,j,k} + A_i\ DX_{i,j,k}$$
$$+ B_k\ EX_{i,j,k} + B_k\ FX_{i,j,k} + E_{i,j,k}) + A_i\ CX_{i,j,k}$$
$$T^{n+1}_{i,j+1,k} + A_i\ DX_{i,j,k}\ T^{n+1}_{i,j-1,k} = G_{i,j,k} - E_{i,j,k}\ T^{n}_{i,j,k} \quad (17)$$
$$- A_i\ AX_{i,j,k}\ T^{n+1}_{i+1,j,k} - A_i\ BX_{i,j,k}\ T^{n+1}_{i-1,j,k} - B_k\ EX_{i,j,k}\ T^{n+1}_{i,j,k+1}$$
$$- B_k\ FX_{i,j,k}\ T^{n+1}_{i,j,k-1}$$

If we let all terms to the right of the equal sign equal $H_{i,j,k}$ and define the coefficient of $T^{n+1}_{i,j,k}$ as Del′, then:

$$- T^{n+1}_{i,j,k}\ Del' + A_i\ CX_{i,j,k}\ T^{n+1}_{i,j+1,k} + A_i\ DX_{i,j,k}\ T^{n+1}_{i,j-1,k} = H_{i,j,k} \quad (18)$$

The system of equations as presented in the form of equation (18) is then solved using the Thomas algorithm for tridiagonal matrices. (For explanation of the algorithm, see Smith, 1965; Von Rosenberg, 1969.)

Introducing X and Y as coefficients in the Thomas algorithm, we obtain:

$$T^{n+1}_{i,j-1,k} = X_{j-1}\ T^{n+1}_{i,j,k} + Y_{j-1} \quad (19)$$

and substituting equation (19) into equation (18) we obtain:

$$- Del'\ T^{n+1}_{i,j,k} = H_{i,j,k} - A_i\ CX_{i,j,k}\ T^{n+1}_{i,j+1,k} - A_i\ DX_{i,j,k}\ X_{j-1}\ T^{n+1}_{i,j,k}$$
$$- A_i\ DX_{i,j,k}\ Y_{j-1} \quad (20)$$

solving for $T^{n+1}_{i,j,k}$ yields:

$$T^{n+1}_{i,j,k} = - \frac{(H_{i,j,k} - A_i\ DX_{i,j,k}\ Y_{j-1} - A_i\ CX_{i,j,k}\ T^{n+1}_{i,j+1,k})}{Del' - A_i\ DX_{i,j,k}\ X_{j-1}} \quad (21)$$

letting $Del = Del' - A_i\ DX_{i,j,k}\ X_{j-1}$

then:

$$T^{n+1}_{i,j,k} = \frac{A_i\ CX_{i,j,k}\ T^{n+1}_{i,j+1,k} + A_i\ DX_{i,j,k}\ Y_{j-1} - H_{i,j,k}}{Del} \quad (22)$$

since

$$T^{n+1}_{i,j,k} = X_j\ T^{n+1}_{i,j+1,k} + Y_j \quad (23)$$

$$X_j = \frac{A_i\ CX_{i,j,k}}{Del} \quad (24)$$

$$Y_j = \frac{A_i\ DX_{i,j,k}\ Y_{j-1} - H_{i,j,k}}{Del} \quad (25)$$

After a solution for T^{n+1} is obtained in a given row, the next row in the same layer is solved. After a solution is produced for each layer, the routine proceeds to solve the next lower layer in the same manner. This procedure continues until a complete block of space is solved at the n+1 time step (see Fig. 1 and 2). When a T^{n+1} time level is solved (the entire grid is satisfied for some sigma), the time step is increased as: $\Delta t^{n+2} = \phi \Delta t^{n+1}$ where ϕ ranges from 1. to about 6. depending upon the boundary conditions and spacing. Time is advanced as: $Time^{n+2} = Time^{n+1} + \Delta t^{n+2}$. The T^{n+1} values are substituted into the T^n array and new T^{n+2} values are solved. This procedure continues until either a predetermined time span is satisfied or until the number of computation cycles is satisfied.

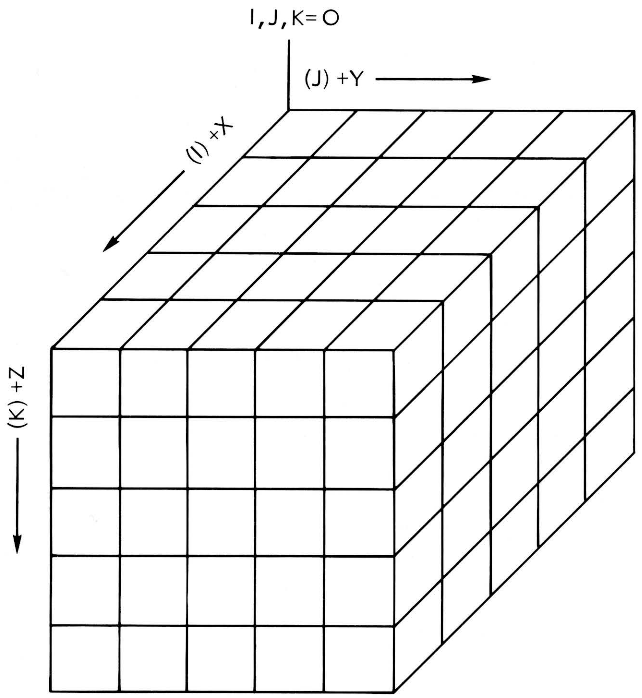

FIGURE 1.—Coordinate and grid system used in the analysis.

A simple program using the preceding developed coefficients is available (Halepaska and Hartman, 1971) upon request.

The heat flow equation in rz geometry is

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\kappa \frac{\partial T}{\partial r}\right) + \frac{\partial}{\partial y}\left(\kappa \frac{\partial T}{\partial y}\right) + Q = Cp\,\rho \frac{\partial T}{\partial t} \qquad (26)$$

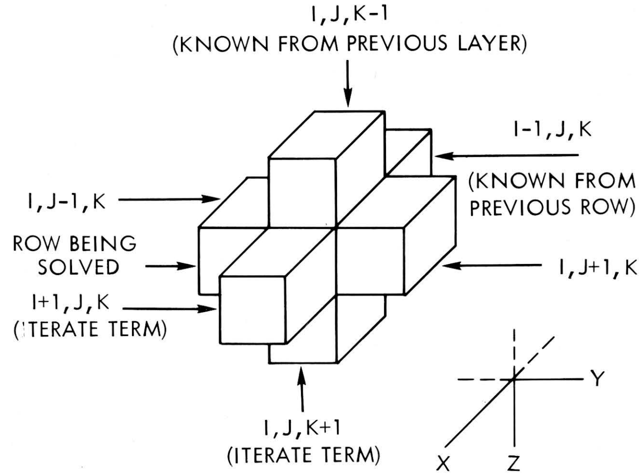

FIGURE 2.—Solution block and coordinate system used in the analysis.

Let $u = \ln \frac{r}{r_w}$, then equation (26) takes the form

$$\frac{e^{-2u}}{r_w^2}\frac{\partial}{\partial u}\left(\kappa \frac{\partial T}{\partial u}\right) + \frac{\partial}{\partial y}\left(\kappa \frac{\partial T}{\partial y}\right) + Q = Cp\,\rho \frac{\partial T}{\partial t} \qquad (27)$$

where u = dimensionless length

r_w = some basic dimension (radius of the source or sink term for example).

Use of the transformation on the radial part of the differential equation allows the investigator to go from line symmetry (r,y) to plane symmetry (x,y) in an efficient manner. It also provides for equal grid spacing in either plane or cylindrical symmetry.

The same procedures outlined in the differencing of the 3-dimensional equation hold for equation (27).

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