## 5 - Fast Methods for 1D USS HC Problems

The previous introductory methods of solving heat transfer problems have required that the following time-step constraints must be observed to avoid instability and divergence in the numerical solution:

- 1D USS HC $$\frac{\alpha\Delta t}{\Delta x^2} \leq \frac{1}{2} \tag{5.1}$$
- 2D USS HC $$\frac{\alpha\Delta t}{\Delta x^2} \leq \frac{1}{4} \tag{5.2}$$
- 3D USS HC $$\frac{\alpha\Delta t}{\Delta x^2} \leq \frac{1}{6} \tag{5.3}$$

This chapter presents *fast methods* for one-dimensional problems. Two of the methods are explicit: Saul'yev and the DuFort-Frankel Methods. A third method, the Crank-Nicolson Method, is an implicit method. It is also the basis of multidimensional fast methods. The Crank-Nicolson Method requires the simultaneous solution of a system of linear equations that have a characteristic form called a *Tridiagonal Matrix*. An algorithm for solving such a system is presented called the *Tridiagonal Matrix Algorithm*. The Crank-Nicolson Method is the first solution method that cannot be solved using Microsoft Excel® without using macro code.

Tutorials are available on the course website that will help one to learn how to write and deploy macros in Microsoft Excel®. The programming language used for writing macros is Visual Basic® and shares many of its features with the stand-alone Visual Basic® application and other .NET applications from Microsoft®. However, the student only needs to be familiar with the elementary elements of Visual Basic® within Microsoft Excel® to succeed in the macro writing part of this course. These macros are also referred to as VBA's

One might hypothesize that the reason for the above limitations in the time step arises from the position mismatch in the positions of the approximations for the position and the time derivatives. For example, in the 1D USS HC solution, the position and time derivatives $\partial^2 T / \partial x^2$ and $\partial T / \partial t$ are centered about (t, x) and (t + $\Delta$t/2, x), respectively, as shown in Figure. 1. Methods are now presented that avoid this mismatch. They allow larger time steps than demanded by Eqs. (5.1) - (5.3).

All of the fast methods presented in this chapter use a modified method of approximating the second partial derivative in the Heat Equation. In the Saul'yev and the DuFort-Frankel Methods, the second partial is approximated from the difference in the two first derivatives $\lambda_2$ and $\lambda_1$ at x+$\Delta$x/2 and x-$\Delta$x/2 such that.

$$\frac{\partial^2 T}{\partial x^2} \approx \frac{\lambda_2 - \lambda_1}{\Delta x} \tag{5.4}$$

The primary difference in the methods is how the two first derivatives, $\lambda_2$ and $\lambda_1$, are selected.

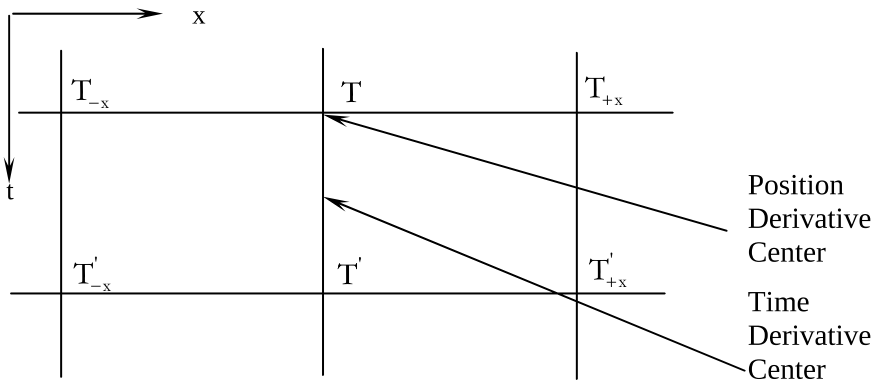



Figure 1. The Relative Positions of the Time and Position Derivatives for Elementary, Explicit 1D USS HT Numerical Solution

## 5.1 Saul'yev Method: 1D USS HT

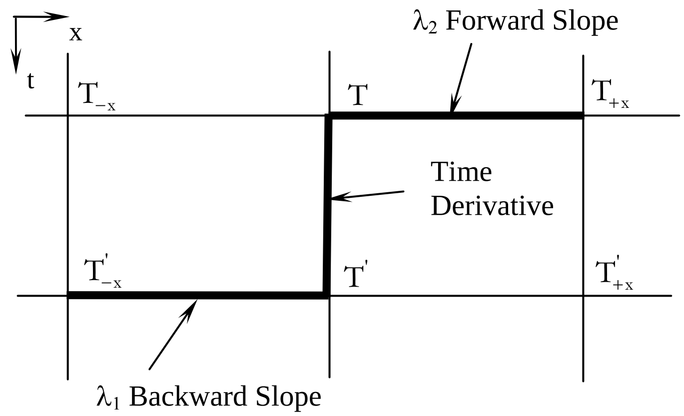
The Saul'yev method uses two different approximations for the position derivative. One approximation is used to calculate from left to right and the second approximation is used to calculate from right to left. Figure 2 shows the fist derivative selections.

The approximation for left-to-right computations is given by Eq. (5.5). The approximation involves two temperatures at the forward time step: $T'$ and $T'_{-x}$. Normally, having two forward (unknown) temperatures in the approximation would make solving for the values of $T'$ at each location across the time step implicit; however, it does not in this case. This is because Eq. (5.5) proceeds from left to right and the value of $T'_{-x}$ is the left boundary value at the first computation. As the computations proceed, each computed $T'$ becomes the next computation's $T'_{-x}$. Therefore, Eq. (5.5) allows the computation of all of the new temperatures at one time step. Of course, the errors from the skewed approximation of the second derivative employed in Eq. (5.5) would accumulate if it were used repetitively for many time steps. The error from this skew is eliminated by reversing the procedure starting at the right boundary using Eq.(5.5)

$$\frac{\partial^2 T}{\partial x^2} \approx \left[ \frac{\dfrac{T_{+x} - T}{\Delta x} - \dfrac{T' - T'_{-x}}{\Delta x}}{\Delta x} \right] \longrightarrow \tag{5.5}$$

$$\frac{\partial^2 T}{\partial x^2} \approx \left[ \frac{\dfrac{T'_{+x} - T'}{\Delta x} - \dfrac{T - T_{-x}}{\Delta x}}{\Delta x} \right] \longleftarrow \tag{5.6}$$

a) Left-to-Right




b) Right-to-Left

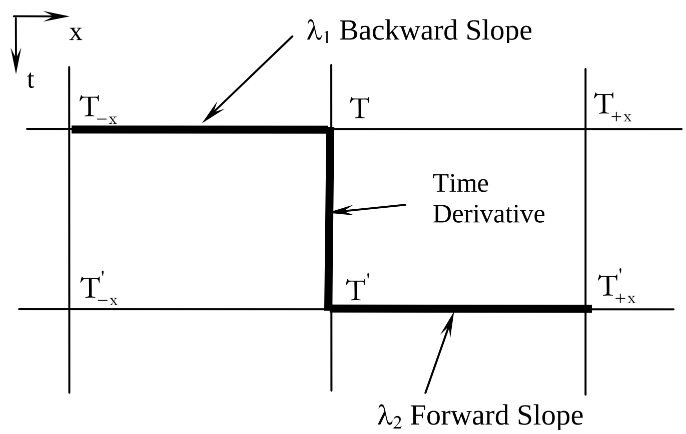



Figure 2. The location of first derivatives used to approximate the Heat Equation in Saul'yev's Method.

The time derivative is the forward difference approximation

$$\frac{\partial T}{\partial t} \approx \frac{T' - T}{\Delta t} \tag{5.7}$$

Substituting these approximations into the Heat Equation

$$\alpha\left[\frac{\partial^2 T}{\partial x^2}\right] = \frac{\partial T}{\partial t} \tag{5.8}$$

gives

$$T' = \frac{T + f\left[T_{+x} + T'_{-x} - T\right]}{1 + f} \qquad \longrightarrow \tag{5.9}$$

$$T' = \frac{T + f\left[T'_{+x} + T_{-x} - T\right]}{1 + f} \qquad \longleftarrow \tag{5.10}$$

where $f = \dfrac{\alpha \Delta t}{\Delta x^2}$.

Eqs. (5.9) and (5.10) are used alternatively to compute each unknown temperature at a given time. The new value of T on the right-hand side of each equation is always known.

## 5.2 - DuFort-Frankel Method

The DuFort-Frankel Method requires knowing the initial temperatures for two previous time steps. Figure 3 shows the selection of first derivatives used to approximate the second derivative as well as the use of the central time derivative. The second derivative in the Heat Equation is then approximated as

$$\frac{\partial^2 T}{\partial x^2} \approx \frac{\dfrac{T_{+x} - {}'T}{\Delta x} - \dfrac{T' - T_{-x}}{\Delta x}}{\Delta x} \tag{5.11}$$

Substituting this approximation and the central approximation of the time derivative into the Heat Equation and solving for T' gives

$$T' = \frac{{}'T + 2f\left[T_{+x} + T_{-x} - {}'T\right]}{1 + 2f} \tag{5.12}$$

The student should verify that the position approximation could have been written as

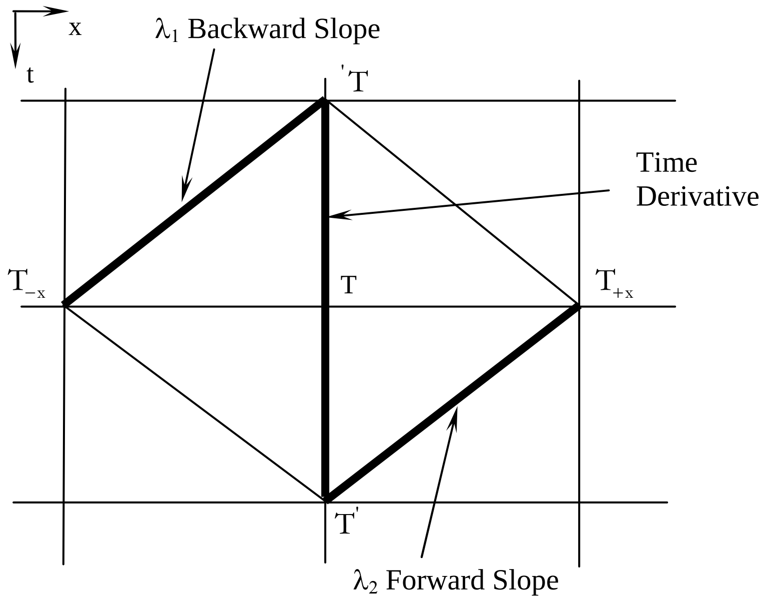
$$\frac{\partial^2 T}{\partial x^2} \approx \frac{\dfrac{T_{+x} - T'}{\Delta x} - \dfrac{{}'T - T_{-x}}{\Delta x}}{\Delta x} \tag{5.13}$$

but this is mathematically identical to Eq. (5.11). Therefore, there is no skew in Eq. (5.12).

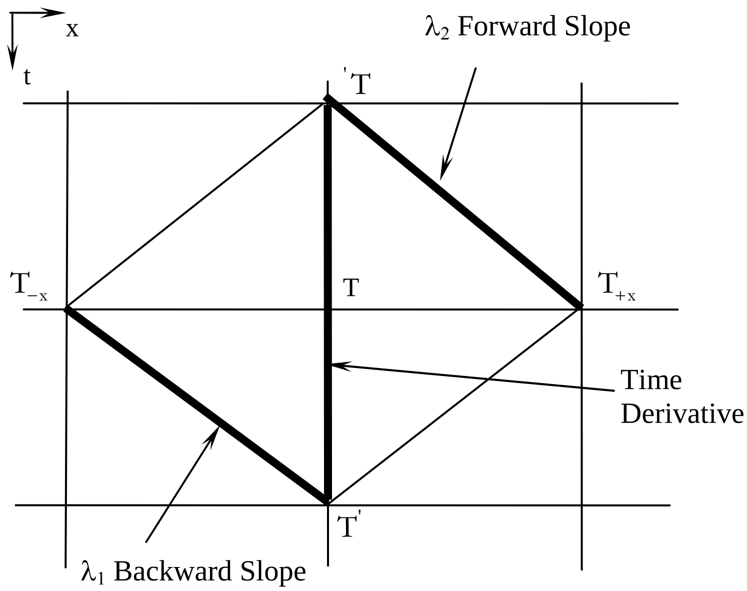
## 5.3 - Crank Nicolson Method

The Crank-Nicolson Method creates a coincidence of the position and the time derivatives by averaging the position derivative for the old and the new temperatures while using the forward derivative for the time derivative. The position derivatives are both central differences centered about (t, x) and (t+Δt/2, x) as shown in Figure 4.




a) Arrangement 1




b) Arrangement 2 – Mathematically the same as Arrangement 1

Figure 3. The Location of First Derivatives in DuFort-Frankel Method.

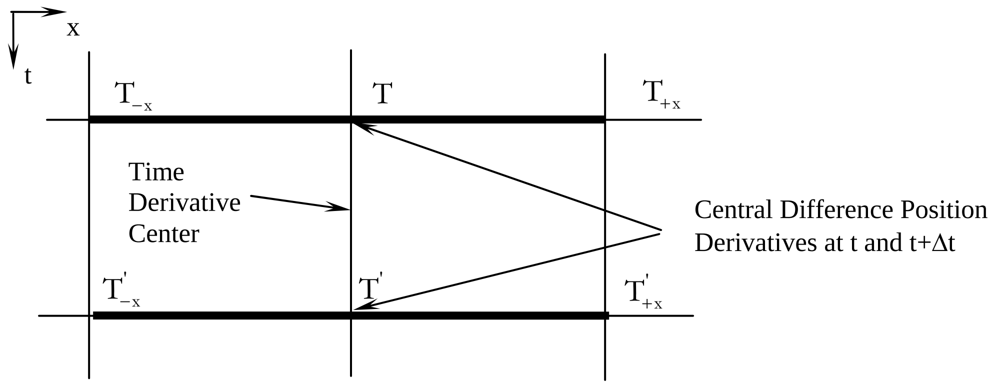



Figure 4. Locations of the time and position derivatives for Crank-Nicolson Method

The Heat Equation

$$\alpha\left[\frac{\partial^2 T}{\partial x^2}\right] = \frac{\partial T}{\partial t} \tag{5.14}$$

then becomes

$$\alpha\left[\frac{\dfrac{\left[T_{+x} - 2T + T_{-x}\right]}{\Delta x^2} + \dfrac{\left[T'_{+x} - 2T' + T'_{-x}\right]}{\Delta x^2}}{2}\right] = \frac{T' - T}{\Delta t} \tag{5.15}$$

There is one such equation for each unknown grid point in the calculation grid that means there are as many equations as unknowns. Therefore, the problem may be solved using Eq. (5.15) but there is a wrinkle heretofore not encountered. That problem is that Eq. (5.15) cannot be explicitly solved for T' since it also contains unknown temperatures $T'_{-x}$ and $T'_{+x}$. Therefore the solution for all the new temperatures for one time requires a simultaneous solution of all expressions of Eq. (5.15) for each grid point at the new time. Of course the boundaries are known.

Eq. (5.15) may be rearranged to give

$$T' - f\left(T'_{-} - 2T' + T'_{+}\right) = T + f\left[\left(T_{-} - 2T + T_{+}\right)\right] \tag{5.16}$$

where $f = \dfrac{\alpha \Delta t}{2\Delta x^2}$

The unknown temperatures at the new time appearing in Eq. (5.16) may be collected as

$$aT'_{-} + bT' + cT'_{+} = fT_{-} + (1-2f)T + fT_{+} \tag{5.17}$$

where

$$a = -f \tag{5.18}$$
$$b = (1+2f) \tag{5.19}$$
$$c = -f \tag{5.20}$$

There are only two unknown temperatures in the equations that are for the grid points one position step in from the two boundaries. All the equations for the remaining grid points will have three unknown temperatures.

If one assumes there are 10 increments and, therefore, 11 grid points in the x direction, there will be nine unknown temperatures and two known boundary temperatures. The new temperatures are denoted as usual as $T_0^{'}, T_1^{'}, T_2^{'}, \ldots T_{10}^{'}$.

The complete enumerations of Eq. (13) for all grid points where the temperatures are unknown are

1. $$bT_1^{'} + cT_2^{'} = fT_0 + (1-2f)T_1 + fT_2 - aT_0^{'} = d_1 \tag{5.21}$$
2. $$aT_1^{'} + bT_2^{'} + cT_3^{'} = fT_1 + (1-2f)T_2 + fT_3 = d_2 \tag{5.22}$$
3. $$aT_2^{'} + bT_3^{'} + cT_4^{'} = fT_2 + (1-2f)T_3 + fT_4 = d_3 \tag{5.23}$$
4. $$aT_3^{'} + bT_4^{'} + cT_5^{'} = fT_3 + (1-2f)T_4 + fT_5 = d_4 \tag{5.24}$$
5. $$aT_4^{'} + bT_5^{'} + cT_6^{'} = fT_4 + (1-2f)T_5 + fT_6 = d_5 \tag{5.25}$$
6. $$aT_5^{'} + bT_6^{'} + cT_7^{'} = fT_5 + (1-2f)T_6 + fT_7 = d_6 \tag{5.26}$$
7. $$aT_6^{'} + bT_7^{'} + cT_8^{'} = fT_6 + (1-2f)T_7 + fT_8 = d_7 \tag{5.27}$$
8. $$aT_7^{'} + bT_8^{'} + cT_9^{'} = fT_7 + (1-2f)T_8 + fT_9 = d_8 \tag{5.28}$$
9. $$aT_8^{'} + bT_9^{'} = fT_8 + (1-2f)T_9 + fT_{10} - cT_{10}^{'} = d_9 \tag{5.29}$$

which gives the coefficient matrix, which may be very easily and efficiently solved using the Tridiagonal Matrix Algorithm.

Table 1. Tridiagonal Coefficient Matrix

| Eq. | $T_1$' | $T_2$' | $T_3$' | $T_4$' | $T_5$' | $T_6$' | $T_7$' | $T_8$' | $T_9$' | RHS |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | b | c | | | | | | | | $d_1$ |
| 2 | a | b | c | | | | | | | $d_2$ |
| 3 | | a | b | c | | | | | | $d_3$ |
| 4 | | | a | b | c | | | | | $d_4$ |
| 5 | | | | a | b | c | | | | $d_5$ |
| 6 | | | | | a | b | c | | | $d_6$ |
| 7 | | | | | | a | b | c | | $d_7$ |
| 8 | | | | | | | a | b | c | $d_8$ |
| 9 | | | | | | | | a | b | $d_9$ |

## 5.4 -Tridiagonal Matrix Algorithm

Crank-Nicolson has all the same a's, b's, and c's and are not subscripted. The general Tridiagonal Algorithm allows unique values of a, b, and c in each equation and are, therefore, subscripted.

$$T_N = \gamma_N \tag{5.30}$$

$$T_i = \gamma_i - \frac{c_i T_{i+1}}{\beta_i} \qquad i = N-1,\ N-2,\ ....1 \tag{5.31}$$

where the β's and γ's are determined from the recursion formulas

$$\beta_1 = b_1 \tag{5.32}$$

$$\gamma_1 = d_1 / \beta_1 \tag{5.33}$$

$$\beta_i = b_i - \frac{a_i c_{i-1}}{\beta_{i-1}} \qquad i = 2,\ \ 3,\ \ ......,\ \ N \tag{5.34}$$

$$\gamma_i = \frac{d_i - a_i \gamma_{i-1}}{\beta_i} \qquad i = 2,\ \ 3,\ \ ......,\ \ N. \tag{5.35}$$

## 5.5 – Saul'yev with Convection and Fixed Flux Boundary Conditions

The above Saul'yev rectilinear formulation for a problem with 10 increments assumes that the boundary temperatures are known fixed values: $T_0$ and $T_{10}$. It is common to encounter fixed flux and convection boundary conditions in which cases there arises a computational conflict at the boundary if either $T_0'$ or $T_{10}'$ are required in the computation of $T'$. This occurs because for a fixed flux or convection boundary condition, these values are determined from $T'$ creating a circular computation. This may be avoided by substituting the boundary equation into the Saul'yev equation at grid columns 1 and 9 as now shown.

*Fixed flux*: Eq. [4.4] describes the boundary temperature for a fixed flux condition. When written in terms of the Saul'yev notation for the two boundaries, it becomes

$$T_0' = T_1' + \frac{q_{fixed}}{k}\Delta x \tag{5.36}$$

and

$$T_{10}' = T_9' + \frac{q_{fixed}}{k}\Delta x \tag{5.37}$$

where $q_{fixed}$ is a scalar quantity equaling the heat leaving the surface. The Saul'yev formulations Eq. [5.9] for $T_1'$ $T_1$ and Eq. [5.10] for $T_9'$ may be written

$$T_1' = \frac{T_1 + f\left[T_2 + T_0' - T_1\right]}{1+f} \tag{5.38}$$

$$T_9' = \frac{T_9 + f\left[T_{10}' + T_8 - T_9\right]}{1+f} \tag{5.39}$$

where $f = \dfrac{\alpha \Delta t}{\Delta x^2}$

Substituting Eq. (5.36) into Eq. (5.38) and Eq. (5.37) into Eq. (5.39) gives

$$T_1' = \frac{T_1 + f\left[T_2 + \left(T_1' + q_{fixed}\frac{\Delta x}{k}\right) - T_1\right]}{1+f} \tag{5.40}$$

and

$$T_9' = \frac{T_9 + f\left[\left(T_9' + q_{fixed}\frac{\Delta x}{k}\right) + T_8 - T_9\right]}{1+f} \tag{5.41}$$

Solving for $T_1'$ or $T_9'$ gives

$$T_1' + = T_1 + f\left[T_2 - T_1 + q_{fixed}\frac{\Delta x}{k}\right] \tag{5.42}$$

and

$$T_9' = T_9 + f\left[T_8 - T_9 + q_{fixed}\frac{\Delta x}{k}\right] \tag{5.43}$$

The zero flux condition is a special case of the fixed flux: $q_{fixed} = 0$.

*Convection Boundary*: For a convection boundary condition, Eq. (4.7) is used rather than Eq. (4.4). The equations corresponding to Eqs. (5.36) and (5.37) are

$$T_0' = \frac{T_a h + T_1'(k/\Delta x)}{h + (k/\Delta x)} = \frac{T_a + cT_1'}{1+c} \tag{5.44}$$

and

$$T_{10}' = \frac{T_a h + T_9'(k/\Delta x)}{h + (k/\Delta x)} = \frac{T_a + cT_9'}{1+c} \tag{5.45}$$

where $c = \dfrac{k}{h\Delta x}$.

Solving Eq. (5.44) into Eq. (5.38) and solving for $T_1'$ gives

$$T_1' = \frac{fT_a + (1+c)\left(T_1 + f\,(T_2 - T_1)\right)}{1+c+f} \tag{5.46}$$

and

$$T_9^{'} = \frac{fT_a + (1+c)\left(T_9 + f\left(T_8 - T_9\right)\right)}{1+c+f} \tag{5.47}$$

## 5.6 - Crank-Nicolson with Convection Boundary at the Surface and Zero Flux

The above rectilinear formulation assumes that the boundary temperatures are known fixed values: $T_0$ and $T_{10}$. In practice, it is more likely to encounter a convection condition or, if symmetry permits, a zero flux boundary. Each of these conditions is considered below as is the use of cylindrical and spherical coordinates.

*Convection in Rectilinear Coordinates*: Convection at a boundary requires that the temperature at the surface is the temperature that balances the convection flux from the surface with the conduction flux to the surface. Since the surface cannot store energy, these fluxes may be set equal and solved for the needed surface temperature as now shown for rectilinear coordinates.

When the left boundary, for example, is made a convection condition with the fluid at $T_a$, then $T_o$ becomes a function of $T_1$ given by

$$T_0 = \left(hT_a + \left(k/\Delta x\right)T_1\right)\Big/\left(h + k/\Delta x\right) = \frac{1}{1 + k/h\Delta x}T_a + \frac{1}{1 + h\,\Delta x/k}T_1 \tag{5.48}$$

This equation holds for both old and new temperatures. Therefore, Eq. (5.16) becomes

$$-\frac{f}{(1+c)}\left(T_a + T_1^{'}\right) + (1+2f)T_1^{'} - fT_2^{'} = \frac{f}{(1+c)}\left(T_a + T_1\right) + (1-2f)T_1 - fT_2 \tag{5.49}$$

$$\left[1 + f\left(\frac{1+2c}{(1+c)}\right)\right]T_1^{'} - fT_2^{'} = \left[1 - f\left(\frac{1+2c}{(1+c)}\right)\right]T_1 - fT_2 + \frac{2f}{(1+c)}T_a = d_1 \tag{5.50}$$

where $c = \dfrac{k}{h\Delta x}$.

*Zero Flux in Rectilinear Coordinates*: For a zero flux condition at the right side, $T_{10}$ becomes an unknown written in terms of $T_9$ and $T_{11}$, which is the same as $T_9$ because of the symmetry at the boundary. Therefore, a tenth equation is added to Eqs. (5.21)– (5.29)

10. $$2\,aT_9^{'} + bT_{10}^{'} = -2\,fT_9 + (2\text{f-}1)T_{10} = d_{10} \tag{5.51}$$

*Radial Coordinates:* When the conduction is occurring in a solid described in radial coordinates and additional first order term appears on the direction-side of the Heat Equation as shown in Eq. (5.12).

$$\alpha\left[\frac{\partial^2 T}{\partial r^2} + \frac{g}{r}\frac{\partial T}{\partial r}\right] = \frac{\partial T}{\partial t} \tag{5.52}$$

where g is 0, 1, or 2 for rectilinear, cylindrical, or spherical coordinates.

In the Crank-Nicolson method this additional term is approximated as

$$\frac{g}{r}\left[\frac{\left(\frac{T_+ - T_-}{2\Delta r}\right)+\left(\frac{T_+^{'} - T_-^{'}}{2\Delta r}\right)}{2}\right] \tag{5.53}$$

This makes the coefficients for a, b, c, and d without convection or a zero flux boundary the following:

$$a = -f(1-\frac{g\Delta r}{2r}) \tag{5.54}$$

$$b = (1+2f) \tag{5.55}$$

$$c = -f(1+\frac{g\Delta r}{2r}) \tag{5.56}$$

$$\mathrm{d} = \mathrm{f}(1+\frac{\mathrm{g}\Delta \mathrm{r}}{2\mathrm{r}})\mathrm{T}_- + (1-2\mathrm{f})\mathrm{T} + \mathrm{f}(1-\frac{\mathrm{g}\Delta \mathrm{r}}{2\mathrm{r}})\mathrm{T}_+ \tag{5.57}$$

The reader should be able to use the above concepts to write the appropriate expressions for convection in radial coordinates.