Appendix H

NUMERICAL TECHNIQUES

This appendix shows the various numerical techniques that can be employed in solving design problems, which could pose difficulty if an analytical method is used. The numerical methods can readily be incorporated into computer programs to obtain results of design problems.

H.1 SIMPSON'S RULE FOR AREA UNDER THE CURVE

Simpson's rule is a numerical integration technique that is widely used in calculating the area under the curve. It is simple and has a greater degree of accuracy than the trapezoidal rule. The Simpson's 1/3 rule is based on quadratic polynomial interpolation.

Figure H-1 shows a section of a curve and three coordinates erected to it at equally spaced intervals along the x-axis. Simpson's rule states that the area P′PQQ′ is given approximately by the formula

$$\text{Area} = \frac{h}{3}(y_1 + 4y_2 + y_3) \tag{H-1}$$

If we reduce the step size h, the result becomes more accurate. The interval over which the integral is to be taken is divided into larger number of equal sub intervals as shown in Figure H-2.

We will divide the total area into four sections, namely P′PRR′, R′RSS′, S′STT′, and T′TQQ′.

We shall write down the expression for each area and sum them up to obtain the total area P′PQQ′.

$$\text{Area of P′PRR′} = \frac{h}{3}(y_1 + 4y_2 + y_3) \tag{H-2}$$

$$\text{Area of R′RSS′} = \frac{h}{3}(y_3 + 4y_4 + y_5) \tag{H-3}$$

$$\text{Area of S′STT′} = \frac{h}{3}(y_5 + 4y_6 + y_7) \tag{H-4}$$

$$\text{Area of T′TQQ′} = \frac{h}{3}(y_7 + 4y_8 + y_9) \tag{H-5}$$

The total area is the sum of the areas P′PRR′, R′RSS′, S′STT′, and T′TQQ′.

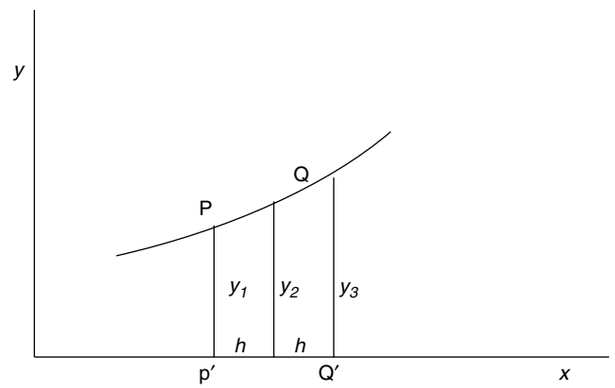

Figure H-1

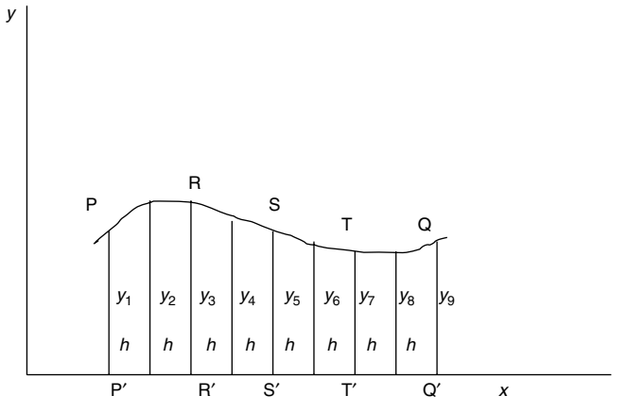

Figure H-2

$$\begin{aligned}\text{Total area} &= \frac{1}{3}h\,(y_1 + 4y_2 + y_3 + y_3 + 4y_4 + y_5 + y_5 + 4y_6 \\ &\quad + y_7 + y_7 + 4y_8 + y_9) \\ &= \frac{1}{3}h\,[y_1 + 4(y_2 + y_4 + y_6 + y_8) + 2(y_3 + y_5 + y_7) \\ &\quad + y_9]\end{aligned} \tag{H-6}$$

The Simpson's 1/3 rule for a quadratic integrated over two Δx intervals that are of uniform width or panel is

$$\begin{aligned}\text{Area} = I &= \int_a^b f(x)\,\mathrm{d}x \\ &= \frac{h}{3}(y_1 + 4y_2 + 2y_3 + 4y_4 + 2y_5 + \cdots \\ &\quad + 2y_{n-1} + 4y_n + y_{n+1}) + E \\ &= \text{width} \times \text{average height}\end{aligned} \tag{H-7}$$

SIMPSON'S 3/8 RULE

Simpson's 3/8 rule is derived by integrating a third-order polynomial interpolation formula. For a domain (a, b) divided into three intervals, it is expressed as

$$\begin{aligned}\text{Area} = I &= \int_a^b f(x)\,\mathrm{d}x = \frac{3h}{8}(y_1 + 3y_2 + 3y_3 + 2y_4 + 3y_5 + \\ &\quad + 3y_6 + \cdots + 2y_{n-2} + 3y_{n-1} + 3y_n + y_{n+1}) + E \\ &= \text{width} \times \text{height}\end{aligned} \tag{H-8}$$

EXAMPLE H-1

A tracer experiment was carried out in a nozzle type reactor of volume $V = 5.13\,\text{L}$ with liquid rate at 2.9 L/min. Table H-1 shows data for the exit age distribution $E(\theta)$ against the dimensionless residence time θ. Determine the area under the distribution curve.

TABLE H-1

θ	$E(\theta)$	θ	$E(\theta)$
0.000	0.000	1.243	0.403
0.113	0.308	1.356	0.355
0.226	0.995	1.469	0.313
0.339	0.876	1.582	0.275
0.452	0.786	1.695	0.237
0.565	0.720	1.808	0.213
0.678	0.663	1.921	0.171
0.791	0.606	2.034	0.142
0.904	0.545	2.147	0.123
1.017	0.497	2.260	0.109
1.130	0.450	2.373	0.095

(*Source*: A.K. Coker, Ph.D., *Study of Fast Reactions in Nozzle Type Reactors*, Aston Univ., Birmingham, UK, 1985.)

A computer program PROG7 has been developed to determine the area under the distribution curve from the residence time distribution function $E(t)$ and expressed as follows:

$$\int_0^\infty E(t)\,\mathrm{d}t = 1 \tag{H-9}$$

The average time spent by material flowing at a rate q through a volume V

$$\text{equals } \bar{t} = \frac{V}{q} \tag{H-10}$$

We can also express Eq. (H-9) in the form of dimensionless time where

$$\theta = \frac{tq}{V} \tag{H-11}$$

and this becomes

$$\int_0^\infty E(\theta)\,\mathrm{d}\theta = 1 \tag{H-12}$$

Using the Excel spreadsheet program prog7a.xls or Fortran program PROG7, the area under the residence time distribution of the tracer response can be calculated. Table H-1 shows the computer results of the program, and Figure H-3 shows a residence time distribution from a tracer experiment studying the mixing characteristics of a nozzle type reactor that behaves non-ideally [1].

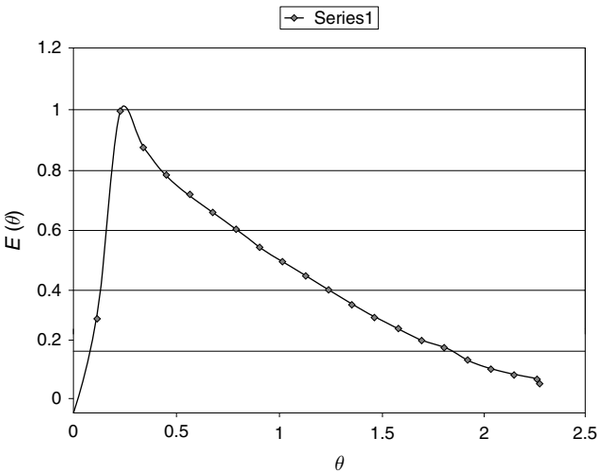

Figure H-3 Residence time distribution to a tracer response.

A computer program PROG7 has been developed to determine the area under the curve. Simpson's rule is also easy to use in Microsoft Excel spreadsheet. We can carry this out by entering the x-values in one column, the y-values in the next column. We then follow this procedure by an additional column containing the y-values multiplied by their appropriate constants (i.e., multiplied by 4 or 2, except the initial and final values). We sum the last column to obtain the value of the integral and multiply this by $\Delta x/3$.

H.2 NON-LINEAR EQUATIONS

The Newton–Raphson's iterative method is a process for the determination of a real root of an equation $f(x) = 0$, given just one point close to the desired root (Figure H-4). If we let x_0 represent the known approximate value of the root of $f(x) = 0$, and h be the difference between the true value α and the approximate value, we have

$$\alpha = x_0 + h$$

From Taylor series,

$$f(x) = f(x_0) + hf'(x_0) + \frac{h}{2!}f''(x_0) + \cdots + \frac{h}{n!}f^n(x_0) \tag{H-13}$$

about x_0, gives

$$f(\alpha) = f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h}{2!}f''(\xi) \tag{H-14}$$

where

$\xi = x_0 + \theta h, 0 < \theta < 1$, lies between α and x_0. Ignoring the remainder term and writing $f(\alpha) = 0$, we have

$$f(x_0) + hf'(x_0) \approx 0 \tag{H-15}$$

so that

$$h \approx -\frac{f(x_0)}{f'(x_0)} \tag{H-16}$$

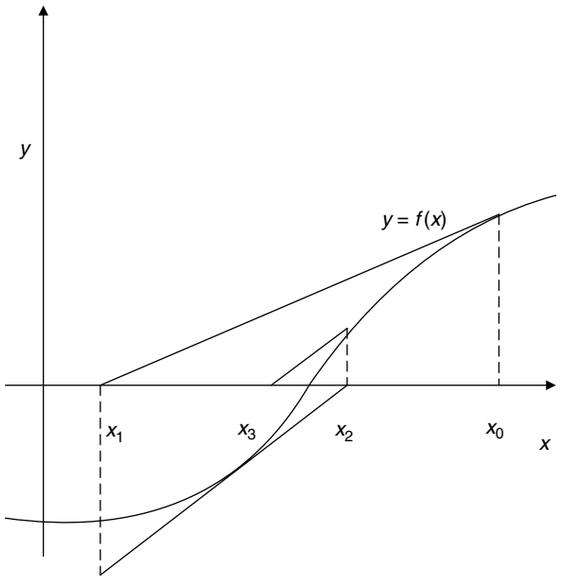

Figure H-4 Newton–Raphson's method.

Therefore, the next root that gives a better estimate than x_0 is

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} \tag{H-17}$$

Better approximations may be obtained by repetition (iteration) of the process. We may write this as

$$\mathrm{x}_{n+1} = \mathrm{x}_n - \frac{f(x_n)}{f'(x_n)} \tag{H-18}$$

Each iteration provides the point at which the tangent at the original point cuts the x-axis as shown in Figure H-4. The equation of the tangent at the point $[x_n, f(x_n)]$ is

$$y - f(x_n) = f'(x_n)(x - x_n) \tag{H-19}$$

Therefore the point $(x_{n+1}, 0)$ corresponds to

$$-f(x_n) = f'(x_n)(x_{n+1} - x_n) \tag{H-20}$$

which gives

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \tag{H-21}$$

A developed computer program PROG6.FOR is used to solve non-linear (e.g., Colebroke–White) equation using Newton–Raphson's method of iteration in Chapter 9.

SOLUTION OF NON-LINEAR EQUATIONS

Consider a set of N non-linear equations of the form

$$\begin{aligned} F(x, y, \dots) &= 0 \\ G(x, y, \dots) &= 0 \end{aligned} \tag{H-22}$$

where $x, y, \dots$ are the roots of the N equations. These equations can be solved explicitly for the roots. If we consider some points (x_1, y_1) near the root of definition for the functions F, G, we can expand both functions by an N-dimensional Taylor series about the point (x_1, y_1) as

$$\begin{aligned} F(x, y, \dots) = 0 = F(x_1, y_1 \dots) &+ \frac{\partial F}{\partial x}\Big|_0 (x - x_1) \\ &+ \frac{\partial F}{\partial y}\Big|_0 (y - y_1) + \cdots \\ G(x, y, \dots) = 0 = G(x_1, y_1 \dots) &+ \frac{\partial G}{\partial x}\Big|_0 (x - x_1) \\ &+ \frac{\partial G}{\partial y}\Big|_0 (y - y_1) + \cdots \end{aligned} \tag{H-23}$$

Truncating the series after the first-order derivative and rewriting in matrix form will yield

$$\begin{bmatrix} \frac{\partial F}{\partial x}|_0 & \frac{\partial F}{\partial y}|_0 \cdots \\ \frac{\partial G}{\partial x}|_0 & \frac{\partial G}{\partial y}|_0 \cdots \\ \vdots & \end{bmatrix} \begin{bmatrix} x - x_1 \\ y - y_1 \\ \vdots \end{bmatrix} = \begin{bmatrix} F - F_0 \\ G - G_0 \\ \vdots \end{bmatrix} \tag{H-24}$$

We can solve for the roots $x, y, \dots$ which give $F = G = \dots = 0$ as

$$\begin{bmatrix} x \\ y \\ \vdots \end{bmatrix} = \begin{bmatrix} x_1 \\ y_1 \\ \vdots \end{bmatrix} - \begin{bmatrix} \frac{\partial F}{\partial x}|_0 & \frac{\partial F}{\partial y}|_0 \cdots \\ \frac{\partial G}{\partial x}|_0 & \frac{\partial G}{\partial y}|_0 \cdots \\ \vdots & \end{bmatrix}^{-1} \begin{bmatrix} F_0 \\ G_0 \\ \vdots \end{bmatrix} \tag{H-25}$$

for $N = 1$

Equation (H-25) becomes

$$x = x_1 - \frac{F_0}{\frac{\partial F}{\partial x}|_0} \tag{H-26}$$

This is Newton–Raphson's method for finding the roots of an equation.

When $N = 2$

$$\begin{aligned} x &= x_1 - \frac{F_0 \frac{\partial G}{\partial x}\big|_0 - G_0 \frac{\partial F}{\partial x}\big|_0}{\frac{\partial F}{\partial x}\big|_0 \cdot \frac{\partial G}{\partial y}\big|_0 - \frac{\partial F}{\partial y}\big|_0 \cdot \frac{\partial G}{\partial x}\big|_0} \\ y &= y_1 - \frac{-F_0 \frac{\partial G}{\partial y}\big|_0 + G_0 \frac{\partial F}{\partial y}\big|_0}{\frac{\partial F}{\partial x}\big|_0 \cdot \frac{\partial G}{\partial y}\big|_0 - \frac{\partial F}{\partial y}\big|_0 \cdot \frac{\partial G}{\partial x}\big|_0} \end{aligned} \tag{H-27}$$

Equation (H-27) is a two-dimensional generalization of Newton's method. This technique is often employed to solve large sets of non-linear algebraic equations. Care must be taken in choosing initial guess (x_1, y_1) quite close to the final roots, as the algorithm may diverge. A developed computer program PROG8 is used to solve non-linear equations as illustrated by the following example.

The computer program PROG8 can be used to solve any number of non-linear equations. The partial derivatives of the functions are estimated by the difference quotients when a variable is perturbed by an amount equal to a small value (Δ) used in the program to perturb the X-values. Table H-2 shows the computer results of Example H-2.

H.3 SOLUTION OF SIMULTANEOUS, FIRST-ORDER, ORDINARY DIFFERENTIAL EQUATIONS

Analytical solutions to complex kinetic reactions in reactor systems are time-consuming and intractable. The designer must resort to

EXAMPLE H-2

A pair of reactions $A + B \xrightarrow{k_1} 2C$ and $A + C \xrightarrow{k_2} D$ are conducted in a four-stage continuous flow stirred tank reactors (CFSTR) with $C_{AO} = 0.9\,\text{mol/m}^3$, $C_{BO} = 0.3\,\text{mol/m}^3$, and $C_{CO} = C_{DO} = 0\,\text{mol/m}^3$. The residence time in each stage is 10 min. Determine the exit concentrations of *A* and *B* in the four CFSTRs. The rate expressions are

$$(-r_A) = k_1\, C_A\, C_B + k_2\, C_A\, C_C \text{ and } (-r_B) = k_1\, C_A\, C_B\,\text{mol/m}^3\,\text{min}$$

where

$k_1 = 0.3\,\text{m}^3/\text{mol min}$
$k_2 = 0.15\,\text{m}^3/\text{mol min}$.

Solution

Figure H-5 shows a battery of CFSTR with $C_{AO} = 0.9\,\text{mol/m}^3$ and $C_{BO} = 0.3\,\text{mol/m}^3$ in the first tank and where, $V_1 = V_2 = V_3 = V_4 = V_R$, u = volumetric flow rate, and the residence time, $\bar{t} = V_R/u = 10\,\text{min}$.

General mass balance

Input by flow = output by flow + disappearance by reaction + accumulation

Assuming that the operation is at steady state and, therefore, accumulation = 0

Mass balance on first CFSTR

The material balance on species A is:

$$uC_{A0} = uC_{A1} + (k_1\, C_{A1}\, C_{B1} + k_2\, C_{A1}\, C_C)\, V_R \tag{H-28}$$

The stoichiometry between species A, B, and C is

$$C_C = 3(C_{B0} - C_B) - (C_{A0} - C_C)$$
$$= 0.9 - 3C_B - 0.9 + C_A$$
$$C_C = C_A - 3C_B \tag{H-29}$$

Substituting Eq. (H-29) into Eq. (H-28) gives

$$C_{A0} = C_{A1} + C_{A1}\,\bar{t}\,[k_1\, C_{B1} + k_2(C_{A1} - 3C_{B1})]$$

or

$$0.9 = C_{A1} + 3C_{A1}\, C_{B1} + 1.5\, C_{A1}(C_{A1} - 3C_{B1}) \tag{H-30}$$

Material balance on species B is

$$uC_{B0} = uC_{B1} + k_1\, C_{A1}\, C_{B1}\, V_R \tag{H-31}$$

or

$$0.3 = C_{B1} + 3C_{A1}C_{B1} \tag{H-32}$$

Second CFSTR Material balance on species A is

$$uC_{A1} = uC_{A2} + [k_1\, C_{A2}C_{B2} + k_2\, C_{A2}(C_{A2} - 3C_{B2})]V_R \tag{H-33}$$

or

$$C_{A1} = C_{A2} + 10[0.3\, C_{A2}\, C_{B2} + 0.15\, C_{A2}(C_{A2} - 3C_{B2})] \tag{H-34}$$

Material balance on species B is

$$uC_{B1} = uC_{B2} + k_1\, C_{A2}\, C_{B2}\, V_R \tag{H-35}$$

or

$$C_{B1} = C_{B2} + 3C_{A2}C_{B2} \tag{H-36}$$

Rearranging Eq (H-35) and (H-36) yields

$$C_{A2} + 3C_{A2}C_{B2} + 1.5C_{A2}(C_{A2} - 3C_{B2}) = C_{A1}$$
$$C_{B2} + 3C_{A2}C_{B2} = C_{B1} \tag{H-37}$$

Third CFSTR

The material balances on species A and B are

$$C_{A3} + 3C_{A3}C_{B3} + 1.5C_{A3}(C_{A3} - 3C_{B3}) = C_{A2}$$
$$C_{B3} + 3C_{A3}C_{B3} = C_{B2} \tag{H-38}$$

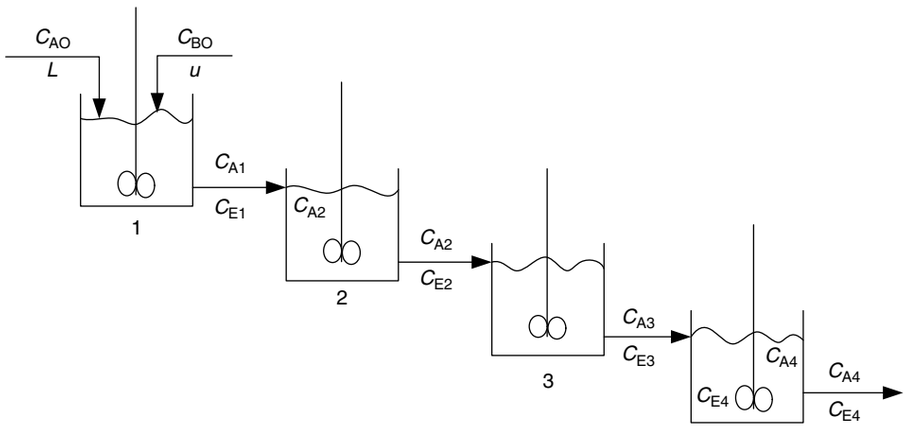

Figure H-5 A battery of CFSTR.

(*continued*)

EXAMPLE H-2 —(*continued*)

Fourth CFSTR
The material balances on species A and B are

$$C_{A4} + 3C_{A4}C_{B4} + 1.5C_{A4}(C_{A4} - 3C_{B4}) = C_{A3}$$

$$C_{B4} + 3C_{A4}C_{B4} = C_{B3} \tag{H-39}$$

These are eight non-linear equations involving the material balances of species A and B in the four stirred tank reactors. Rearranging these equations yields the following:

$$\begin{aligned}
1.5C_{A1}{}^2 - 1.5C_{A1}C_{B1} + C_{A1} - 0.9 &= 0 \\
3C_{A1}C_{B1} + C_{B1} - 0.3 &= 0 \\
1.5C_{A2}{}^2 - 1.5C_{A2}C_{B2} + C_{A2} - C_{A1} &= 0 \\
3C_{A2}C_{B2} + C_{B2} - C_{B1} &= 0 \\
1.5C_{A3}{}^2 - 1.5C_{A3}C_{B3} + C_{A3} - C_{A2} &= 0 \\
3C_{A3}C_{B3} + C_{B3} - C_{B2} &= 0 \\
1.5C_{A4}{}^2 - 1.5C_{A4}C_{B4} + C_{A4} - C_{A3} &= 0 \\
3C_{A4}C_{B4} + C_{B4} - C_{B3} &= 0
\end{aligned} \tag{H-40}$$

A computer program PROG8 was developed using the Newton–Raphson's method to determine the outlet concentration of species A and B from the four stirred tank reactors. The eight equations (Eqs H-40) are supplied as functions in the subroutine of PROG8 as

$$F(1) = 1.5 * X(1) * X(1) - 1.5 * X(1) * X(2) + X(1) - 0.9$$

$$F(2) = 3.0 * X(1) * X(2) + X(2) - 0.3$$

$$F(3) = 1.5 * X(3) * X(3) - 1.5 * X(3) * X(4) + X(3) - X(1)$$

$$F(4) = 3.0 * X(3) * X(4) + X(4) - X(2)$$

$$F(5) = 1.5 * X(5) * X(5) - 1.5 * X(5) * X(6) + X(5) - X(3)$$

$$F(6) = 3.0 * X(5) * X(6) + X(6) - X(4)$$

$$F(7) = 1.5 * X(7) * X(7) - 1.5 * X(7) * X(8) + X(7) - X(5)$$

$$F(8) = 3.0 * X(7) * X(8) + X(8) - X(6) \tag{H-41}$$

where

$$C_{A1} = X(1), C_{B1} = X(2), C_{A2} = X(3), C_{B2} = X(4)$$
$$C_{A3} = X(5), C_{B3} = X(6), C_{A4} = X(7), C_{B4} = X(8).$$

The exit concentrations of species A and B from the computer results and the initial guesses of

$C_{A1} = 0.1, C_{B1} = 0.1, C_{A2} = 0.1, C_{B2} = 0.1, C_{A3} = 0.1, C_{B3} = 0.1, C_{A4} = 0.1, C_{B4} = 0.1$, are as follows.

$C_{A1} = X(1) = 0.54599$ $C_{B1} = X(2) = 0.11372$
$C_{A2} = X(3) = 0.3703$ $C_{B2} = X(4) = 0.05386$
$C_{A3} = X(5) = 0.2718$ $C_{B3} = X(6) = 0.02958$
$C_{A4} = X(7) = 0.21107$ $C_{B4} = X(8) = 0.01792.$

TABLE H-2 Newton Method For Solving Non-linear Equations

```
Initial roots

X(1)= 0.1000
X(2)= 0.1000
X(3)= 0.1000
X(4)= 0.1000
X(5)= 0.1000
X(6)= 0.1000
X(7)= 0.1000
X(8)= 0.1000

Final roots

X(1)= 0.54599
X(2)= 0.11372
X(3)= 0.37030
X(4)= 0.05386
X(5)= 0.27180
X(6)= 0.02958
X(7)= 0.21107
X(8)= 0.01792
```

numerical techniques with the aid of a computer for his or her solutions. The reactions taking place in batch and piston flow reactions involve a set of simultaneous, first-order, ordinary differential equations. Several numerical methods have been used for solving sets of equations, and the most popular method is the Runge–Kutta fourth order. The Runge–Kutta is a powerful integration technique that can be easily implemented on a personal computer. The only drawback is its instability if the step size is too large. In a set of equations, the Runge–Kutta algorithm uses the same step size for each member of the set of equations. This causes practical problems if the set is *stiff* where some members of these equations have characteristic times much smaller than other members of the equations. An example is the free-radical kinetics reaction, which has rates that may differ by three orders of magnitude.

In general, a system of nth first-order equations will be of the form

$$\frac{dy_i}{dx} = f_i(x, y_o, y_1, y_2, \ldots, y_{n-1}), \quad i = 0, 1, 2, 3, \ldots, n \tag{H-42}$$

with n initial conditions $y_i(X_0) = A_i, \quad i = 0, 1, 2, \ldots, n$

Consider the system of two equations:

$$\frac{dy}{dx} = f(x, y, z) y(x_0) = y_0 \tag{H-43}$$

$$\frac{dz}{dx} = g(x, y, z) z(x_0) = z_0 \tag{H-44}$$

We may advance the solution of y and z to new values at $x_1 = x_0 + h$ using any of the one-step or Runge–Kutta methods.

In general, our solutions will be advanced using expressions of the form

$$y(x_1) = y(x_0) + K \tag{H-45}$$

$$z(x_1) = z(x_0) + L \tag{H-46}$$

where the nature of K or L depends on the method being applied. For the Runge–Kutta fourth order

$$K = \frac{K_1 + 2K_2 + 2K_3 + K_4}{6} \tag{H-47}$$

and

$$L = \frac{L_1 + 2L_2 + 2L_3 + L_4}{6} \tag{H-48}$$

where

$$K_1 = hf(x_0, y_0, z_0) \tag{H-49}$$

$$L_1 = hg(x_0, y_0, z_0) \tag{H-50}$$

$$K_2 = hf\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}K_1, + z_0 + \frac{1}{2}L_1\right) \tag{H-51}$$

$$L_2 = hg\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}K_1, z_0 + \frac{1}{2}L_1\right) \tag{H-52}$$

$$K_3 = hf\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}K_2, z_0 + \frac{1}{2}L_2\right) \tag{H-53}$$

$$L_3 = hg\left(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}K_2, z_0 + \frac{1}{2}L_2\right) \tag{H-54}$$

$$K_4 = hf\,(x_0 + h, y_0 + K_3, z_0 + L_3) \tag{H-55}$$

$$L_4 = hg(x_0 + h, y_0 + K_3, z_0 + L_3) \tag{H-56}$$

H.4 EXTENSION OF RUNGE–KUTTA METHODS

RUNGE–KUTTA–GILL METHOD

The Runge–Kutta–Gill method is the most widely used single-step method for solving ordinary differential equations. For the differential equation

$$\frac{\mathrm{d}y}{\mathrm{d}x} = f(x, y), y(x_n) = y_n \tag{H-57}$$

$$y_{n+1} = y_n + \frac{1}{6}\left[k_1 + 2\left(1 - \frac{1}{\sqrt{2}}\right)\mathrm{k}_2 + 2\left(1 + \frac{1}{\sqrt{2}}\right)\mathrm{k}_3 + \mathrm{k}_4\right] + \mathrm{O}(h^5) \tag{H-58}$$

where

$$\begin{aligned}
k_1 &= hf(x_i, y_i)\\
k_2 &= hf\left(x_i + \frac{h}{2}, y_i + \frac{1}{2}k_1\right)\\
k_3 &= hf\left(x_i + \frac{h}{2}, y_i + \left[\frac{-1}{2} + \frac{1}{\sqrt{2}}\right]k_1 + \left[1 - \frac{1}{\sqrt{2}}\right]k_2\right)\\
k_4 &= hf\left(x_i + h, y_i - \frac{1}{\sqrt{2}}k_2 + \left[1 + \frac{1}{\sqrt{2}}\right]k_3\right)
\end{aligned} \tag{H-59}$$

THE RUNGE–KUTTA–MERSON METHOd

The Runge–Kutta–Merson method outlines a process for deciding the step size for better predetermined accuracy. For this method, five functions are evaluated at every step. The algorithm is

$$\begin{aligned}
k_1 &= h\mathrm{f}(x_i, y_i)\\
k_2 &= h\mathrm{f}\left(x_i + \frac{h}{3}, y_i + \frac{k_1}{3}\right)\\
k_3 &= h\mathrm{f}\left(x_i + \frac{h}{3}, y_1 + \frac{k_1}{6} + \frac{k_2}{6}\right)\\
k_4 &= h\mathrm{f}\left(x_i + \frac{h}{2}, y_i + \frac{k_1}{8} + \frac{3k_3}{8}\right)\\
k_5 &= h\mathrm{f}\left(x_i + h, y_i + \frac{k_1}{2} - \frac{3k_3}{2} + 2k_4\right)
\end{aligned}$$

$$y_{n+1} = y_n + \frac{1}{6}(k_1 + 4k_4 + k_5) + \mathrm{O}(h^5) \tag{H-60}$$

We can estimate the local error from a weighted sum of the individual estimate.

$$E = \frac{1}{30}(2k_1 - 9k_3 + 8k_4 - k_5) \tag{H-61}$$

The following Example H-3 illustrates the use of Runge–Kutta fourth order with the Excel spreadsheet.

H.5 PARTIAL DIFFERENTIAL EQUATION

If two or more independent variables are involved in a differential equation, we can express the differential equation as partial differential equation (PDE).

We shall consider the second-order equation (PDE) of the form

$$A\frac{\partial^2 u}{\partial x^2} + B\frac{\partial^2 u}{\partial x \partial y} + C\frac{\partial^2 u}{\partial y^2} + D\left(x, y, u, \frac{\partial u}{\partial x}, \frac{\partial u}{\partial y}\right) = 0 \tag{H-65}$$

where the coefficients *A, B, C*, and *D* are functions of *x, y*, and *u; x* and *y* are the independent variables and *u* is the dependent variable. We can classify Eq. (H-65) with respect to the sign of the discriminant $\Delta = (B^2 - 4AC)$. The equation is elliptical if $\Delta < 0$, hyperbolic if $\Delta > 0$, and parabolic type if $\Delta = 0$.

ELLIPTICAL EQUATION

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -u \tag{H-66}$$

and the Laplace equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \tag{H-67}$$

The coefficients $A = C = 1, B = 0$ and $B^2 - 4AC = -4$ are examples of elliptical equation.

HYPERBOLIC EQUATION

The wave equation

$$\frac{\partial^2 u}{\partial t^2} = \frac{Tg}{w}\frac{\partial^2 u}{\partial x^2} \tag{H-68}$$

is a hyperbolic type where the coefficients $A = 1, B = 0, C = -1$ and $B^2 - 4AC = 4$

PARABOLIC EQUATION

The heat conduction equation

$$\frac{\partial u}{\partial t} = \frac{k}{c\rho}\frac{\partial^2 u}{\partial x^2} \tag{H-69}$$

is a parabolic type where the coefficients $A = 0, B = 0, C = 1$ and $B^2 - 4AC = 0$.

A method for solving the above partial differential equations is to replace the derivatives by difference quotients; that is, converting the equation to a difference equation. We can then write the difference equation that corresponds to each point at the intersections (nodes) of a grid work that subdivides the region of interest at which the function values are known. Solving these equations

EXAMPLE H-3

Consider the dynamic response of component A in a CFSTR undergoing a first-order reaction represented by

$$(-r_A) = kC_A \left(\frac{\text{mol}}{\text{dm}^3\ \text{min}}\right)$$

The rate constant decay is

$$k = k_o - at^2\ (\text{min}^{-1})$$

The first-order differential equation from the mass balance is:

$$\frac{dC_A}{dt} = \frac{u}{V_R}C_{A0} - \left(\frac{u}{V_R} + k_o - at^2\right)C_A \qquad \text{(H-62)}$$

Spreadsheet programming: The Excel program (Prog8a.xls) is used to create numerical solutions using the fourth-order Runge–Kutta by rearranging the above equation to yield

$$\Delta C_A = C_A - C_{A0} = \left[\frac{uC_{A0}}{V_R} - \left(\frac{u}{V_R} + k_o - at^2\right)C_A\right]\Delta t \qquad \text{(H-63)}$$

The transient response concentration C_A is

$$C_A = C_{A0} + \left[\frac{uC_{A0}}{V_R} - \left(\frac{u}{V_R} + k_o - at^2\right)C_A\right]\Delta t \qquad \text{(H-64)}$$

Figure H-6 shows the spreadsheet snap shot of the numerical Runge–Kutta method. Further details are given by Coker, A.K. (*Hydroc. Proc.*, Dec 2004, pp. 77–85).

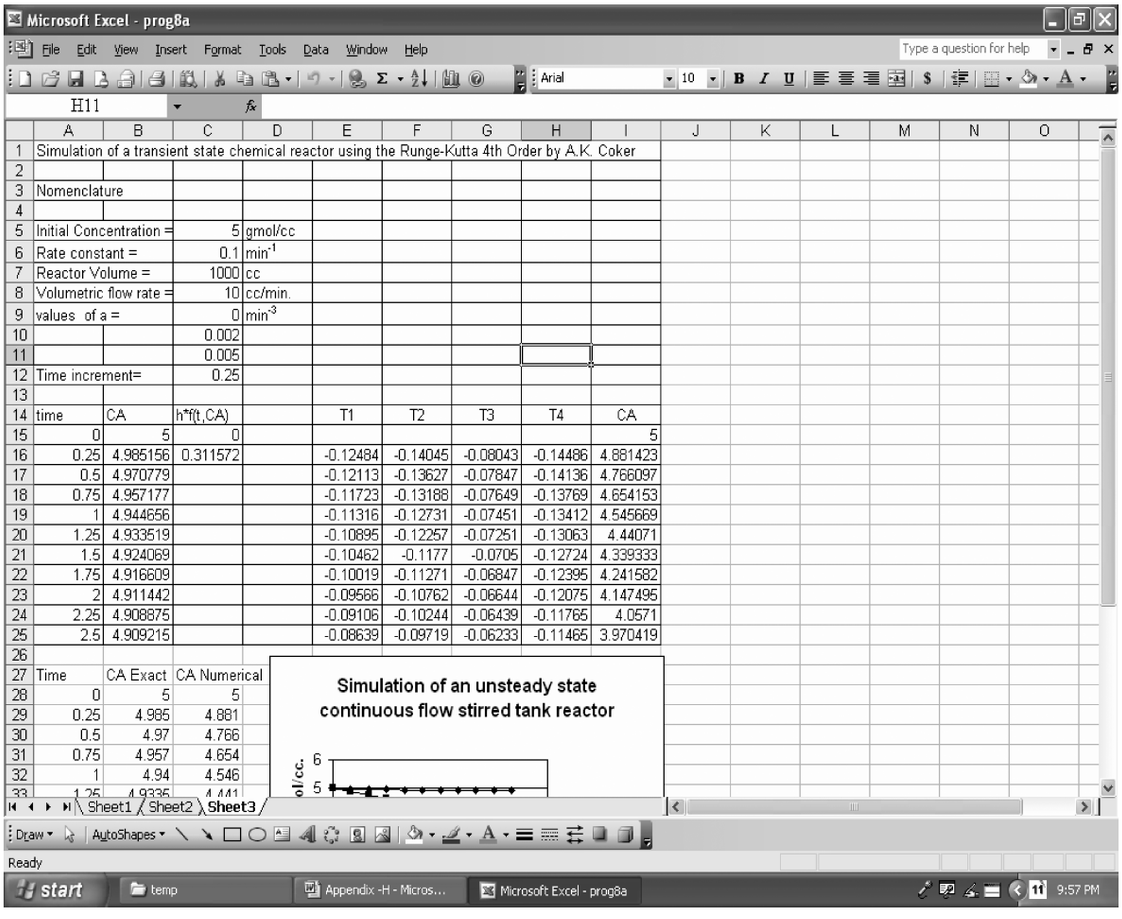

Figure H-6 Simul ation of CFSTR reaction with the Excel program.

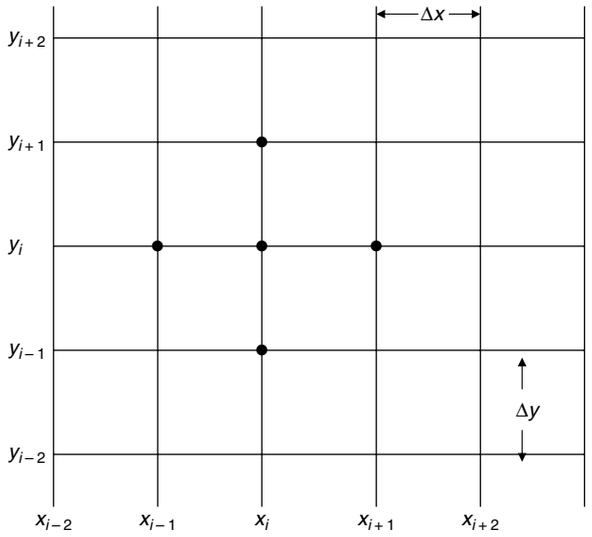

Figure H-7

simultaneously gives values for the function at each node that approximates the true values.

Let $h = \Delta x$ equal spacing of grid work in the x – direction as shown in the Figure H-7.

From Taylor series,

$$f(x_n + h) = f(x_n) + f'(x_n)h + \frac{f''(x_n)h^2}{2} + \frac{f'''(x_n)h^3}{6} + \frac{f''''(x_n)h^4}{24} + \ldots \text{ for } x_n < \xi_1 < x_n + h \tag{H-70}$$

and

$$f(x_n + h) = f(x_n) - f'(x_n)h + \frac{f''(x_n)h^2}{2} - \frac{f'''(x_n)h^3}{6} + \frac{f''''(x_n)h^4}{24} + \ldots \text{ for } x_n - h < \xi_2 < x_n \tag{H-71}$$

It follows that

$$f(x_n + h) + f(x_n - h) = 2f(x_n) + f''(x_n)h^2 + \frac{f''''(\xi)}{12}h^2 \tag{H-72}$$

or

$$f''(x_n) + \frac{f''''(\xi)h^2}{12} = \frac{f(x_n + h) - 2f(x_n) + f(x_n - h)}{h^2} \text{ for } x_n - h < \xi < x_n + h \tag{H-73}$$

Using the subscript notation, we have

$$\mathrm{f}''(x_n) + \mathrm{O}(h^2) = \frac{f_{n+1} - 2f_n + f_{n+1}}{h^2} \tag{H-74}$$

where the subscripts of f indicate the x-values at which it is evaluated. The order relation $\mathrm{O}(h^2)$ shows that error approaches proportionality to h^2 as $h \to 0$.

Similarly, the first derivative is approximated to

$$f(x_n + h) - f(x_n - h) = 2f'(x_n)h + \mathrm{O}(h^2) \tag{H-75}$$

or

$$f'(x_n) = \frac{f(x_n + h) - f(x_n - h)}{2h} \tag{H-76}$$

$$= \frac{f_{n+1} - f_{n-1}}{2h} \tag{H-77}$$

The first derivative could also be approximated by the forward or backward difference, but would have an error of $\mathrm{O}(h)$. The central difference approximation gives the more accurate approximation.

When f is a function of both x and y, we can obtain the second partial derivative with respect to x, $\frac{\partial^2 u}{\partial x^2}$, by holding y constant and evaluating the function at three points where x equals x_n, $x_n + h$, and $x_n - h$. Correspondingly, the partial derivative $\frac{\partial^2 u}{\partial y^2}$ is determined by holding x constant.

Consider the Laplace equation on a region in the xy plane. We subdivide the region with equispaced lines parallel to the x- and y-axes. Consider the region near (x_i, y_i).

$$\nabla^2 u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \tag{H-78}$$

We can replace the derivatives by difference quotients which approximate the derivatives at point (x_i, y_i). Then we have

$$\nabla^2 u(x_i, y_i) = \frac{u(x_{i+1}, y_i) - 2u(x_i, y_i) + u(x_{i-1}, y_i)}{\Delta x^2} + \frac{u(x_i, y_{i+1}) - 2u(x_i, y_i) + u(x_i, y_{i-1})}{\Delta^2 y} = 0 \tag{H-79}$$

or

$$\nabla^2 u_{i,j} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{(\Delta x)^2} + \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{(\Delta y)^2} = 0 \tag{H-80}$$

If we let $\Delta x = \Delta y = h$, the PDE becomes

$$\nabla^2 u_{i,j} = \frac{1}{h^2}\left(u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{i,j}\right) = 0 \tag{H-81}$$

This is known as the standard five-point formula, as five points are involved in the relationship of Eq. (H-81) which points to the right, left, above, and below the central point (x_i, y_i). We can write Eq. (H-81) as

$$u_{i,j} = \frac{1}{4}\left(u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1}\right) \tag{H-82}$$

Instead of Eq. (H-82), we may also use the formula

$$u_{i,j} = \frac{1}{4}\left(u_{i-1,j-1} + u_{i+1,j-1} + u_{i+1,j+1} + u_{i-1,j+1}\right) \tag{H-83}$$

Therefore, the general procedure is to approximate the PDE by a finite difference transformation and then to obtain the solution at the mesh points, using the finite difference approximations. Other numerical methods of solution are the implicit Crank–Nicolson method or the alternating direction implicit scheme (ADI) by Peaceman and Rachford. Details of these methods are illustrated in Numerical analysis texts.

H.6 THE EXPLICIT METHOD

The explicit method divides space and time into discrete uniform subintervals and replaces both time and space derivatives by finite difference approximations, permitting one to easily compute values of the function at a time Δt after the initial time. These values are then used to compute a second set of values and the process is repeated. An approach to solving parabolic partial differential equations by a numerical method is to replace the partial derivatives by finite-difference approximations. An example is the one-dimensional heat flow equation.

$$\frac{\partial^2 u}{\partial x^2} = \frac{c\rho}{k}\frac{\partial u}{\partial t} \tag{H-84}$$

We can use the relations

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{\substack{x = x_i \\ t = t_j}} = \frac{u_{i+1}{}^j - 2u_i{}^j + u_{i-1}{}^j}{(\Delta x)^2} + \mathrm{O}(\Delta x)^2 \tag{H-85}$$

and

$$\left.\frac{\partial u}{\partial t}\right|_{\substack{x = x_i \\ t = t_j}} = \frac{u_i{}^{j+1} - u_i{}^j}{\Delta t} + \mathrm{O}(\Delta t) \tag{H-86}$$

The subscripts are used to denote the position and superscripts for time.

Substituting Eqs (H-85) and (H-86) into Eq. (H-84) and solving for $\mathrm{u}_i{}^{j+1}$ gives the equation for the forward-difference method:

$$u_i{}^{j+1} = \frac{\mathrm{k}\Delta t}{c\rho(\Delta x)^2}\left(u_{i+1}{}^j - u_{i-1}{}^j\right) + \left(1 - \frac{2k\Delta t}{c\rho(\Delta x)^2}\right)u_i{}^j \tag{H-87}$$

Solving for $u_i{}^{j+1}$ in terms of the temperatures at time t_j in Eq. (H-87) for a parabolic partial-differential equation involves subdividing the length into uniform subintervals and applying the finite-difference approximation to Eq. (H-84) at each point where u is not known. Eq. (H-87) then gives the values of u at each interior point at $t = t_1$ since the values at $t = t_0$ are given by the initial conditions. It can be used to get values at t_2 using the values at t_1 as initial conditions, so the solution can be stepped forward in time. At the end points, the boundary conditions will determine u.

The relative size of the time and distance steps, Δt and Δx, affects Eq. (H-87). If the ratio of $\Delta t/(\Delta x)^2$ is chosen so that $k\Delta t/c\rho(\Delta x)^2 = \frac{1}{2}$, the equation is simplified in that the last term vanishes and we have

$$u_i{}^{j+1} = \frac{1}{2}(u_{i+1}{}^j + u_{i-1}{}^j) \tag{H-88}$$

If the value $k\Delta t/c\rho(\Delta x)^2$ is chosen as less than one-half, there will be improved accuracy (limited by the errors dependent on the size of Δx). If the value is chosen greater than one-half, which would reduce the number of calculations required to advance the solution through a given interval of time, the phenomenon of instability sets in. An example is used to illustrate the explicit method.

H.7 INITIAL VALUE METHODS

Another method for solving boundary value problems is to treat them like initial value problems. Since a second-order equation can be reduced to two first-order equations, two initial conditions are required. One condition will be known at a boundary: simply assume a value for the other dependent variable at that same boundary, integrate to the other side, and check if the required boundary condition is satisfied. If not, change the initial value and repeat the integration. The result of this method depends upon the skill with which the iterations are employed in the program.

FINITE DIFFERENCE METHOD IN EXCEL

The Microsoft Excel spreadsheet can be used to program the finite difference method and use the "Calculation" feature to handle the circular reference. First, turn off the iteration, prepare the spreadsheet, and then turn the calculation back on. Whether this converges depends upon the initial guess.

Consider a reaction and diffusion in a flat layer with a first-order reaction represented by

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\mathrm{D}\frac{\mathrm{d}c}{\mathrm{d}x}\right) = kc, \text{ with boundary conditions } \frac{\mathrm{d}c}{\mathrm{d}x}(0) = 0, \quad c(R) = c_{\mathrm{o}} \tag{H-89}$$

where

D = diffusivity
c = concentration
x = position (distance).

The idea in the finite difference method is that the differential equation, valid for all x positions, is replaced by a set of equations representing the equation only at the grid points. Using the finite difference method as derived above, the equation at the grid point is

$$\mathrm{D}\frac{c_{i+1} - 2c_i + c_{i-1}}{\Delta \mathrm{x}^2} = kc_i, \text{ where } c_i = c(x_i) \tag{H-90}$$

Re-arranging Eq. (H-90) to the following form gives

$$c_i = \frac{c_{i+1} + c_{i-1}}{(2 + k\Delta x^2/D)} \tag{H-91}$$

Identify the cells (B1, C1, and D1) in the spreadsheet with the value of concentration at a node i as shown below.

A1	B1	C1	D
$k\Delta x^2/D$	c_{i-1}	c_i	c_{i+1}

Put the value of $k\Delta x^2/D$ in cell A1. The equation for cell C1 is represented by Eq. (H-92) as

$$= (D1 + B1)/(2 + \$A\$1) \tag{H-92}$$

Next, copy this equation over a series of cells that correspond to the number of grid points. For the first and last cell (grid point) use a different equation appropriate to the boundary condition. Then turn on the iteration feature to get the solution.

The next step is to resolve the problem using more grid point and a smaller Δx. This entails that the spreadsheet must be programmed, which gives an indication of whether the answer changes much as the mesh is refined. This ensures that the problem is accurately solved.

H.8 FINITE DIFFERENCE METHOD FOR ELLIPTIC EQUATIONS

Consider the heat condition equation with a heat generation term as:

$$k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) = Q \tag{H-93}$$

The finite difference form of Eq. (H-93) is solved on a worksheet by replacing the derivatives with central differences centered on grid point (i, j).

$$\frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{\Delta x^2} + \frac{T_{i,j+1} - 2T_{i,j} + T_{i,j-1}}{\Delta y^2} = \frac{Q}{k} \tag{H-94}$$

where $T_{i,j}$ is the temperature at the ith location in the x-direction and the jth location in the y-direction. Assuming that the grid spacing $\Delta x = \Delta y$, Eq. (H-94) is rearranged as

$$T_{i,j} = \frac{T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1}}{4} - \Delta x^2 \frac{Q}{k} \tag{H-95}$$

The spreadsheet is then arranged as shown below:

A4 – $\Delta x^2 Q/k$		C4 – $T_{i,j-1}$	
	B5 – $T_{i-1,j}$	C5 – $T_{i,j}$	D5 – $T_{i+1,j}$
		C6 – $T_{i,j+1}$	

When the value of $\Delta x^2 Q/k$ is placed in cell A4, the equation for cell C5 is:

$$= (D5 + B5 + C6 + C4)/4 - \$A\$4 \tag{H-96}$$

In the worksheet, the boundaries of the problem are set with the fixed or derivative values of the boundary conditions, and the interior points are set with Eq. (H-96). Then copy this for every internal grid point, set the boundary equations, and turn on the iteration feature to obtain the solution. This is further carried out again with a finer mesh to assess the accuracy. If the heat of generation term depends upon temperature, it is easy to include that complication just by inserting the formula in place of \$A\$4.

EXAMPLE H-4

A large flat steel plate is 2 cm thick. If the initial temperatures (° C) within the plate are given, as a function of the distance from one face, by the equations

$$u = 100x \quad \text{for } 0 \le x \le 1$$
$$u = 100(2 - x) \quad \text{for } 1 \le x \le 2$$

find the temperatures as a function of x and t if both faces are maintained at 0° C [3].

Data:

$k = 0.13\,\text{cal/s cm °C}$

$c = 0.11\,\text{cal/g °C}$

$\rho = 7.8\,\text{g/cm}^3$

Solution

since the plate is large, the lateral flow of heat relative to the flow perpendicular to the faces can be neglected, and therefore Eq. (H-84) is used for heat flow in one direction. In order to use Eq. (H-88) as an approximation to the physical problem, we subdivide the total thickness into an integral number of spaces.

If we use $\Delta x = 0.25$, this gives eight subdivisions. From Eq. (H-88), Δt is fixed by the relation

$$\frac{k\Delta t}{c\rho(\Delta x)^2} = \frac{1}{2}$$

$$\Delta t = \frac{(0.11)(7.8)(0.25)^2}{(2)(0.13)} = 0.206\,\text{s}$$

The boundary conditions are

$$u(0, t) = 0 \qquad u(2, t) = 0$$

The initial conditions are

$$u(x, 0) = 100x \quad \text{for } 0 \le x \le 1$$
$$u(x, 0) = 100(2 - x) \quad \text{for } 1 \le x \le 2$$

The computer program PROG9 uses the simple algorithm of Eq. (H-88), which indicates that at each interior point the temperature at any point at the end of a time step is just the arithmetic average of the temperatures at the adjacent points at the beginning of that time step. The end temperatures are given by the boundary conditions. Because the temperatures are symmetrical on either side of the center line, we calculate only for $x \le 1.0$. The temperature at $x = 1.25$ is the same as at $x = 0.75$. Table H-3 gives the results of the program.

(*continued*)

Example H-4—(*continued*)

TABLE H-3 Potential Values in One Dimension by Explicit Method

```
FOR X = 0.0 TO X=10.0 WITH DELTA X OF 1.000
AT T= 0.000
  20.000
FOR X= 0.0 TO X=10.0 WITH DELTA X OF 1.000
AT T= 0.000
  20.000
FOR X= 0.0 TO X=10.0 WITH DELTA X OF 1.000
AT T= 0.000
  20.000
FOR X= 0.0 TO X=10.0 WITH DELTA X OF 1.000
AT T= 0.000
  20.000
FOR X= 0.0 TO X=10.0 WITH DELTA X OF 1.000
AT T= 0.000
  20.000
FOR X= 0.0 TO X=10.0 WITH DELTA X OF 1.000
AT T= 0.000
  20.000
FOR X= 0.0 TO X=10.0 WITH DELTA X OF 1.000
AT T= 0.000
  20.000
FOR X= 0.0 TO X=10.0 WITH DELTA X OF 1.000
AT T= 0.000
  20.000
FOR X= 0.0 TO X=10.0 WITH DELTA X OF 1.000
AT T= 0.000
  20.000
FOR X= 0.0 TO X=10.0 WITH DELTA X OF 1.000
AT T= 0.000
  20.000
FOR X= 0.0 TO X=10.0 WITH DELTA X OF 1.000
AT T= 0.000
  20.000

VALUES AT T= 0.288
     0.000  15.000  20.000  20.000  20.000  20.000
    20.000  20.000  20.000  40.000 100.000
VALUES AT T= 0.576
     0.000  15.000  20.000  20.000  20.000  20.000
    20.000  20.000  20.000  40.000 100.000
VALUES AT T= 0.863
     0.000  10.938  17.500  19.688  20.000  20.000
    20.000  21.250  30.000  56.250 100.000
VALUES AT T= 1.151
     0.000  10.938  17.500  19.688  20.000  20.000
    20.000  21.250  30.000  56.250 100.000
VALUES AT T= 1.439
     0.000  9.023  15.469  18.691  19.766  20.059
    20.938 25.234  38.125  63.906 100.000
VALUES AT T= 1.727
     0.000  9.023  15.469  18.691  19.766  20.059
    20.938 25.234  38.125  63.906 100.000
VALUES AT T= 2.015
     0.000  7.855  13.965  17.635  19.375  20.443
    22.793 29.476  44.141  68.579 100.000
VALUES AT T= 2.303
     0.000  7.855  13.965  17.635  19.375  20.443
    22.793 29.476  44.141  68.579 100.000
VALUES AT T= 2.590
     0.000  7.048  12.820  16.717  19.083  21.153
    24.997 33.351  48.741  71.808 100.000
```

(continued)

TABLE H-3—(*continued*)

```
VALUES AT T= 2.878
     0.000  7.048  12.820  16.717  19.083  21.153
    24.997 33.351  48.741  71.808 100.000
VALUES AT T= 3.166
     0.000  6.452  11.942  16.007  18.987  22.081
    27.239 36.751  52.380  74.210 100.000
VALUES AT T= 3.454
     0.000  6.452  11.942  16.007  18.987  22.081
    27.239 36.751  52.380  74.210 100.000
VALUES AT T= 3.742
     0.000  6.002  11.280  15.518  19.091  23.134
    29.383 39.705  55.335  76.083 100.000
VALUES AT T= 4.030
     0.000  6.002  11.280  15.518  19.091  23.134
    29.383 39.705  55.335  76.083 100.000
VALUES AT T= 4.317
     0.000  5.666  10.803  15.233  19.364  24.245
    31.380 42.270  57.784  77.591 100.000
VALUES AT T= 4.605
     0.000  5.666  10.803  15.233  19.364  24.245
    31.380 42.270  57.784  77.591 100.000
VALUES AT T= 4.893
     0.000  5.423  10.486  15.124  19.767  25.372
    33.218 44.507  59.845  78.835 100.000
VALUES AT T= 5.181
     0.000  5.423  10.486  15.124  19.767  25.372
    33.218 44.507  59.845  78.835 100.000
VALUES AT T= 5.469
     0.000  5.262  10.304  15.159  20.268  26.488
    34.902 46.469  61.604  79.879 100.000
VALUES AT T= 5.757
     0.000  5.262  10.304  15.159  20.268  26.488
    34.902 46.469  61.604  79.879 100.000
VALUES AT T= 6.044
     0.000  5.168  10.236  15.312  20.838  27.577
    36.445 48.200  63.120  80.767 100.000
VALUES AT T= 6.332
     0.000  5.168  10.236  15.312  20.838  27.577
    36.445 48.200  63.120  80.767 100.000
VALUES AT T= 6.620
     0.000  5.131  10.261  15.557  21.454  28.632
    37.858 49.738  64.440  81.532 100.000
VALUES AT T= 6.908
     0.000  5.131  10.261  15.557  21.454  28.632
    37.858 49.738  64.440  81.532 100.000
VALUES AT T= 7.196
     0.000  5.141  10.361  15.873  22.100  29.646
    39.158 51.111  65.599  82.197 100.000
VALUES AT T= 7.484
     0.000  5.141  10.361  15.873  22.100  29.646
    39.158 51.111  65.599  82.197 100.000
VALUES AT T= 7.771
     0.000  5.189  10.520  16.242  22.762  30.618
    40.355 52.346  66.624  82.781 100.000
VALUES AT T= 8.059
     0.000  5.189  10.520  16.242  22.762  30.618
    40.355 52.346  66.624  82.781 100.000
VALUES AT T= 8.347
     0.000  5.267  10.725  16.649  23.430  31.548
    41.461 53.462  67.538  83.297 100.000
VALUES AT T= 8.635
     0.000  5.267  10.725  16.649  23.430  31.548
    41.461 53.462  67.538  83.297 100.000
```

(continued)

(continued)

EXAMPLE H-4—(*continued*)

TABLE H-3—(*continued*)

```
VALUES AT T= 8.923
     0.000  5.368  10.965  17.083  24.097  32.435
    42.486 54.476  68.358  83.756 100.000
VALUES AT T= 9.211
     0.000  5.368  10.965  17.083  24.097  32.435
    42.486 54.476  68.358  83.756 100.000
VALUES AT T= 9.498
     0.000  5.486  11.231  17.534  24.757  33.281
    43.438 55.401  69.097  84.168 100.000
VALUES AT T= 9.786
     0.000  5.486  11.231  17.534  24.757  33.281
    43.438 55.401  69.097  84.168 100.000
VALUES AT T= 10.074
     0.000  5.618  11.514  17.995  25.405  34.088
    44.326 56.250  69.769  84.539 100.000
VALUES AT T= 10.362
     0.000  5.618  11.514  17.995  25.405  34.088
    44.326 56.250  69.769  84.539 100.000
VALUES AT T= 10.650
     0.000  5.759  11.809  18.459  26.037  34.856
    45.155 57.031  70.381  84.876 100.000
VALUES AT T= 10.938
     0.000  5.759  11.809  18.459  26.037  34.856
    45.155 57.031  70.381  84.876 100.000
VALUES AT T= 11.225
     0.000  5.906  12.110  18.922  26.653  35.587
    45.931 57.754  70.942  85.184 100.000
VALUES AT T= 11.513
     0.000  5.906  12.110  18.922  26.653  35.587
    45.931 57.754  70.942  85.184 100.000
VALUES AT T= 11.801
     0.000  6.056  12.414  19.380  27.250  36.283
    46.659 58.424  71.458  85.465 100.000
VALUES AT T= 12.089
     0.000  6.056  12.414  19.380  27.250  36.283
    46.659 58.424  71.458  85.465 100.000
VALUES AT T= 12.377
     0.000  6.207  12.717  19.830  27.827  36.946
    47.343 59.048  71.935  85.724 100.000
VALUES AT T= 12.665
     0.000  6.207  12.717  19.830  27.827  36.946
    47.343 59.048  71.935  85.724 100.000
VALUES AT T= 12.952
     0.000  6.358  13.017  20.269  28.383  37.577
    47.987 59.629  72.378  85.963 100.000
VALUES AT T= 13.240
     0.000  6.358  13.017  20.269  28.383  37.577
    47.987 59.629  72.378  85.963 100.000
VALUES AT T= 13.528
     0.000  6.508  13.312  20.697  28.918  38.178
    48.594 60.174  72.789  86.185 100.000
VALUES AT T= 13.816
     0.000  6.508  13.312  20.697  28.918  38.178
    48.594 60.174  72.789  86.185 100.000
VALUES AT T= 14.104
     0.000  6.655  13.601  21.112  29.432  38.749
    49.167 60.684  73.173  86.391 100.000
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(continued)

TABLE H-3—(*continued*)

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VALUES AT T= 14.392
     0.000  6.655  13.601  21.112  29.432  38.749
    49.167 60.684  73.173  86.391 100.000
VALUES AT T= 14.967
     0.000  6.800  13.882  21.513  29.925  39.293
    49.709 61.163  73.531  86.583 100.000
VALUES AT T= 15.255
     0.000  6.940  14.154  21.900  30.398  39.811
    50.221 61.613  73.867  86.763 100.000
VALUES AT T= 15.543
     0.000  6.940  14.154  21.900  30.398  39.811
    50.221 61.613  73.867  86.763 100.000
VALUES AT T= 15.831
     0.000  7.076  14.418  22.272  30.850  40.303
    50.705 62.038  74.183  86.931 100.000
VALUES AT T= 16.118
     0.000  7.076  14.418  22.272  30.850  40.303
    50.705 62.038  74.183  86.931 100.000
VALUES AT T= 16.406
     0.000  7.208  14.672  22.630  31.283  40.772
    51.164 62.438  74.480  87.089 100.000
VALUES AT T= 16.694
     0.000  7.208  14.672  22.630  31.283  40.772
    51.164 62.438  74.480  87.089 100.000
VALUES AT T= 16.982
     0.000  7.335  14.917  22.974  31.696  41.218
    51.599 62.817  74.760  87.238 100.000
VALUES AT T= 17.270
     0.000  7.335  14.917  22.974  31.696  41.218
    51.599 62.817  74.760  87.238 100.000
VALUES AT T= 17.558
     0.000  7.457  15.152  23.303  32.091  41.643
    52.012 63.175  75.023  87.378 100.000
VALUES AT T= 17.845
     0.000  7.457  15.152  23.303  32.091  41.643
    52.012 63.175  75.023  87.378 100.000
VALUES AT T= 18.133
     0.000  7.575  15.378  23.618  32.468  42.047
    52.403 63.513  75.273  87.510 100.000
VALUES AT T= 18.421
     0.000  7.575  15.378  23.618  32.468  42.047
    52.403 63.513  75.273  87.510 100.000
VALUES AT T= 18.709
     0.000  7.688  15.594  23.920  32.828  42.431
    52.775 63.834  75.508  87.635 100.000
VALUES AT T= 18.997
     0.000  7.688  15.594  23.920  32.828  42.431
    52.775 63.834  75.508  87.635 100.000
VALUES AT T= 19.285
     0.000  7.796  15.801  24.208  33.171  42.797
    53.128 64.138 75.731  87.752 100.000
VALUES AT T= 19.572
     0.000  7.796  15.801  24.208  33.171  42.797
    53.128 64.138  75.731  87.752 100.000
VALUES AT T= 19.860
     0.000  7.900  16.000  24.483  33.499  43.145
    53.463 64.426  75.942  87.864 100.000
VALUES AT T= 20.148
     0.000  7.900  16.000  24.483  33.499  43.145
    53.463 64.426  75.942  87.864 100.000
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