

# Chapter 19

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## Numerical Methods

### INTRODUCTION

Early in one's career, the engineer/scientist learns how to use equations and mathematical methods to obtain exact answers to a large range of relatively simple problems. Unfortunately, these techniques are often not adequate for solving real-world problems, although the reader should note that one rarely needs exact answers in technical practice. Most real-world applications are usually inexact because they have been generated from data or parameters that are measured, and hence represent only approximations. What one is likely to require in a realistic situation is not an exact answer but rather one having reasonable accuracy from an engineering point of view.

The solution to an engineering or scientific problem usually requires an answer to an equation or equations, and the answer(s) may be approximate or exact. Obviously an exact answer is preferred, but because of the complexity of some equations, exact solutions may not be attainable. Furthermore, to engineers, an answer that is precise may not be necessary and wastes time. For this condition, one may resort to another method that has come to be defined as a numerical method. Unlike the exact solution, which is continuous and in closed form, numerical methods provide an inexact (but often reasonably accurate) solution. The numerical method leads to discrete answers that are almost always acceptable.

The numerical methods referred to above provide a step-by-step procedure that ultimately leads to an answer and a solution to a particular problem. The method usually requires a large number of calculations and is therefore ideally suited for digital computation.

High speed computing equipment has had a tremendous impact on engineering design, scientific computation, and data processing. The ability of computers to handle large quantities of data and to perform mathematical operations described above at tremendous speeds permits the examination of many more cases and more engineering variables than could possibly be handled on the slide rule—the trademark of engineers of yesteryear. Scientific calculations previously estimated in lifetimes of computation time are currently generated in seconds and, in many instances, microseconds.<sup>(1)</sup>

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This chapter is concerned with numerical methods. This subject was taught in the past as a means of providing engineers with ways to solve complicated mathematical expressions that they could not solve otherwise.

A brief overview of numerical methods is given to provide the practicing engineer with some insight into what many of the currently used software packages (MathCad, Mathematica, MatLab, etc.) are actually doing. The authors have not attempted to cover all the topics of numerical methods. Topics that traditionally fall in the domain of this subject include:

Regression analyses (Illustrative Example 19.1)

Differentiation (Illustrative Example 19.2)

Integration (Illustrative Example 19.3)

Simultaneous linear algebraic equations (Illustrative Example 19.4)

Nonlinear algebraic equations (Illustrative Example 19.5)

Ordinary differential equation(s) (Illustrative Example 19.5)

Partial differential equation(s) (Illustrative Example 19.6)

Optimization (Illustrative Example 19.7)

Since detailed treatment of each of the above topics is beyond the scope of this mass transfer text, the reader is referred to the literature<sup>(2-4)</sup> for a more extensive analysis and additional information. The remainder of this chapter consists of an illustrative example section on applications that examine all the topics listed above. Also note that the illustrative examples primarily address mass transfer topics.

## APPLICATIONS

### ILLUSTRATIVE EXAMPLE 19.1

Two component diffusivity data ( $D$ ) for air–water vapor has been extracted from the literature, as presented in Table 19.1. The literature suggests that diffusivity varies with the temperature to the 1.5 power, i.e.,

$$D \propto T^{1.5}$$

Regress<sup>(5)</sup> the above data to a model of the form

$$D = A + B(T)^{1.5}$$

and indicate how well the model fits the data.

**Table 19.1** Diffusivity–Temperature Data

$T, ^\circ\text{C}$	$D, \text{ft}^2/\text{s}$
0	0.22
25.9	0.258
42.0	0.288
59.0	0.305

**SOLUTION:** A regression analysis (employing EXCEL) shows that

$$A = 0.2208$$

$$B = 0.0015$$

so that

$$D = 0.2208 + 0.0015x; \quad x = T^{1.5}$$

with  $D$  in  $\text{ft}^2/\text{s}$  and  $T$  in  $^\circ\text{C}$ . The correlation coefficient is 0.99554, indicating an excellent fit. ■

### ILLUSTRATIVE EXAMPLE 19.2

Refer to Table 19.2. Generate expressions for the benzene concentration gradient,  $dC/dt$ , at  $t = 4.0$  s. Use several differentiation methods.<sup>(6)</sup>

**SOLUTION:**

#### Method 1

The first method consists of choosing any three data points and calculating the slope of the two extreme points. This slope is approximately equal to the slope at the point lying in the middle. The value obtained will be the equivalent of the derivative at that point 4.

Using data points from 3.0 to 5.0,

$$\begin{aligned} \text{Slope} &= \frac{C_5 - C_3}{t_5 - t_3} \\ &= \frac{1.63 - 2.70}{5.0 - 3.0} = -0.535 \end{aligned}$$

#### Method 2

The second method involves taking the average of two slopes. Using the same points chosen above, two slopes are calculated, one for points 3 and 4 and the other for points 4 and 5. Adding the two results and dividing them by two will provide an approximation of the derivative

**Table 19.2** Illustrative Example 19.2 Data

Time (s)	Concentration of benzene (mg/L)
0.0	7.46
1.0	5.41
2.0	3.80
3.0	2.70
4.0	2.01
5.0	1.63
6.0	1.34
7.0	1.17

at point 4. For the points used in this method, the results are:

$$\begin{aligned}\text{Slope}_1 &= \frac{C_4 - C_3}{t_4 - t_3} \\ &= \frac{2.01 - 2.70}{4.0 - 3.0} = -0.69 \\ \text{Slope}_2 &= \frac{C_5 - C_4}{t_5 - t_4} \\ &= \frac{1.63 - 2.01}{5.0 - 4.0} = -0.38 \\ \text{Slope}_{\text{avg}} &= \frac{-0.69 + (-0.38)}{2} = -0.535\end{aligned}$$

### Method 3

Method three consists of using any three data points (in this case the same points chosen before) and fitting a curve to it. The equation for the curve is obtained by employing a second-order equation and solving it with the three data points. The derivative of the equation is then calculated and evaluated at any point (here, point 4 is used):

$$\begin{aligned}C &= 0.155t^2 - 1.775t + 6.63 \\ \frac{dC}{dt} &= 0.31t - 1.775\end{aligned}$$

Evaluated at  $t = 4.0$  s

$$\frac{dC}{dt} = 0.31(4) - 1.775 = -0.535$$

### Method 4

The following method uses the method of least squares. In this case, all data points are used to generate a second-order polynomial equation. This equation is then differentiated and evaluated at the point where the value of the derivative is required. For example, Microsoft Excel can be employed to generate the regression equation. Once all the coefficients are known, the equation has only to be analytically differentiated:

$$\begin{aligned}C &= 0.1626t^2 - 1.9905t + 7.3108 \\ \frac{dC}{dt} &= 0.3252t - 1.9905\end{aligned}$$

Evaluated at  $t = 4.0$  s:

$$\frac{dC}{dt} = 0.3252(4.0) - 1.9905 = -0.6897$$

### Method 5<sup>(7)</sup>

The last two methods are very similar to each other. They are based on five data points used to generate coefficients. For this development, represent  $C$  and  $t$  by  $f$  and  $x$  (as it appeared in the literature<sup>(7)</sup>), respectively.

The fifth method uses five data points to generate a five coefficient (fourth order) model using an equation of the form  $f = A + Bx + Cx^2 + Dx^3 + Ex^4$  equation. This method is known as interpolating. A set of equations is used to evaluate numerical derivatives from the interpolating polynomial. The equations are listed below:

$$f'(x_0) = \frac{(-25f_0 + 48f_1 - 36f_2 + 16f_3 - 3f_4)}{12h} \quad (19.1)$$

$$f'(x_1) = \frac{(-3f_0 - 10f_1 + 18f_2 - 6f_3 + f_4)}{12h} \quad (19.2)$$

$$f'(x_i) = \frac{(f_{i-2} - 8f_{i-1} + 8f_{i+1} - f_{i+2})}{12h} \quad (19.3)$$

$$f'(x_{n-1}) = \frac{(-f_{n-4} + 6f_{n-3} - 18f_{n-2} + 10f_{n-1} + 3f_n)}{12h} \quad (19.4)$$

$$f'(x_n) = \frac{(3f_{n-4} - 16f_{n-3} + 36f_{n-2} - 48f_{n-1} + 25f_n)}{12h} \quad (19.5)$$

where  $h = x_{i+1} - x_i$

$f_i$  = function evaluated at  $i$

For example, the equation obtained for “the five data set” from 1.0 to 5.0 s, i.e.,  $t = 1.0, 2.0, 3.0, 4.0$  and  $5.0$  s, using the equations given above is

$$f(x) = -0.0012x^4 + 0.002x^3 + 0.2616x^2 - 2.34x + 7.467$$

All these equations are evaluated for each value of  $x$  and  $f(x)$ . The value obtained for point 4.0 is  $-0.5448$ .

### Method 6<sup>(7)</sup>

The last method also uses five data points but only three coefficients are generated for a second-order polynomial equation of the form  $f = A + Bx + Cx^2$ . Another set of equations are used to evaluate the derivative at each point using this method. The equations are provided below:

$$f'(x_0) = \frac{(-54f_0 + 13f_1 + 40f_2 + 27f_3 - 26f_4)}{70h} \quad (19.6)$$

$$f'(x_1) = \frac{(-34f_0 + 3f_1 + 20f_2 + 17f_3 - 6f_4)}{70h} \quad (19.7)$$

$$f'(x_i) = \frac{(-2f_{i-2} - f_{i-1} + f_{i+1} + 2f_{i+2})}{10h} \quad (19.8)$$

$$f'(x_{n-1}) = \frac{(6f_{n-4} - 17f_{n-3} - 20f_{n-2} - 3f_{n-1} + 34f_n)}{70h} \quad (19.9)$$

$$f'(x_n) = \frac{(26f_{n-4} - 27f_{n-3} - 40f_{n-2} - 13f_{n-1} + 54f_n)}{70h} \quad (19.10)$$

At point 4.0, the solution for the derivative using this method is  $-0.6897$ .

Comparing all the values obtained for the derivative at  $t = 4.0$  s, it can be observed that the answers are very close to each other. It is important to remember that these are approximate values and that they vary depending on the approach and the number of data points used to generate the equations. ■

**ILLUSTRATIVE EXAMPLE 19.3**

The volume of a reactor undergoing conversion  $X$  for the reactant (the principal component from the bottom of a distillation column) is described by the following integral:

$$V = 6.0 \times 10^{-3} \int_0^{0.45} \frac{(1 - 0.125X)^3 dX}{10^{-4}(1 - X)(1 - 0.5X)^2}; \quad \text{liters}$$

Calculate the volume using the trapezoidal rule method of integration. Discuss the effect of varying the increment in  $\Delta X$  (e.g., if  $\Delta X = 0.45, 0.09, 0.05, 0.01, 0.005, 0.001$ ).<sup>(8)</sup>

**SOLUTION:** An algorithm for the trapezoid rule is given in Figure 19.1. For an increment size of  $\Delta X = 0.45$ , the step size for the reactor volume is:

$$h = X_1 - X_0 = 0.45 - 0.00 = 0.45$$

Evaluate the function at  $X_0$  and  $X_1$ :

$$\begin{aligned} V_0 &= f(X_0) = 6.0 \times 10^{-3} \left[ \frac{(1 - 0.125X)^3 dX}{10^{-4}(1 - X)(1 - 0.5X)^2} \right]_{X=0.0} \\ &= 6.0 \times 10^{-3} \frac{(1)^3}{10^{-4}(1)(1)^2} \\ &= 60 \end{aligned}$$

$$\begin{aligned} V_1 &= f(X_1) = 6.0 \times 10^{-3} \left[ \frac{(1 - 0.125X)^3 dX}{10^{-4}(1 - X)(1 - 0.5X)^2} \right]_{X=0.45} \\ &= 6.0 \times 10^{-3} \frac{[1 - 0.125(0.45)]^3}{10^{-4}(1 - 0.45)[1 - 0.5(0.45)]^2} \\ &= 152.67 \end{aligned}$$

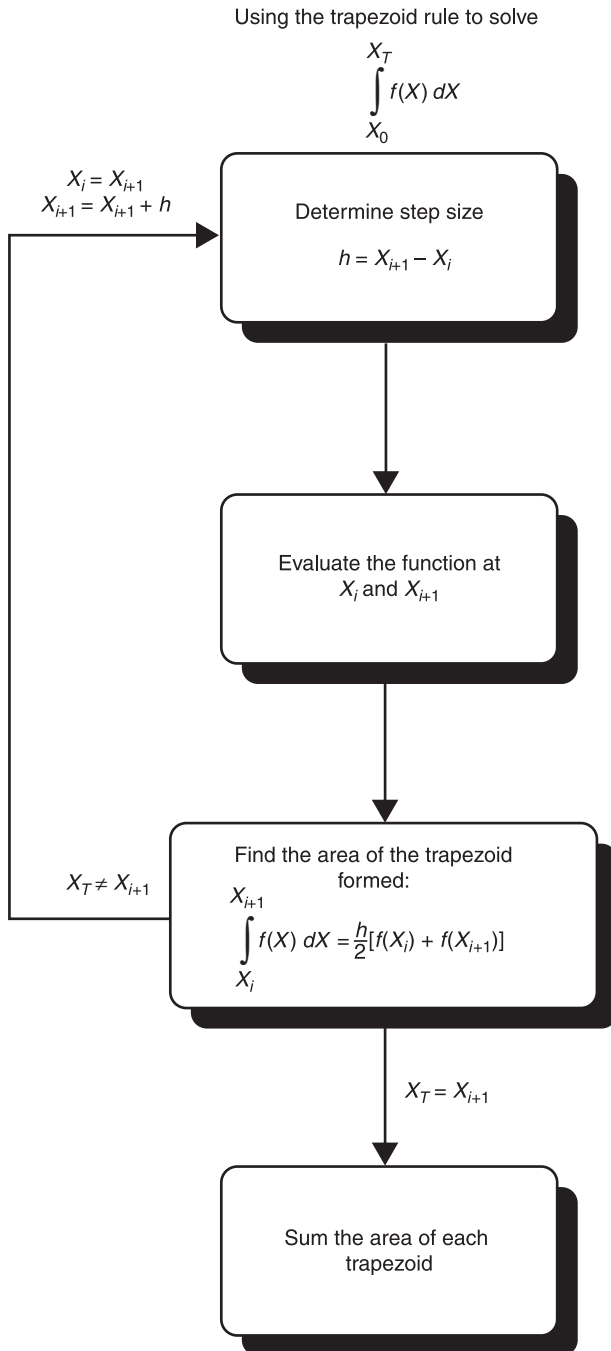
The two-point trapezoid rule is given by

$$\int_{X_0}^{X_1} f(X) dX = \frac{h}{2} [f(X_0) + f(X_1)]$$

Therefore,

$$\begin{aligned} V &= \frac{h}{2} [f(X_0) + f(X_1)] \\ &= \frac{h}{2} [V_0 + V_1] \\ &= \frac{0.45}{2} [60 + 152.67] \\ &= 47.85 \text{ L} \end{aligned}$$

The trapezoid rule is often the quickest but least accurate way to perform a numerical integration by hand. However, if the step size is decreased, the answer should converge to the analytical solution. Note that for smaller step sizes, the results of each numerical integration must be



**Figure 19.1** Algorithm for trapezoid rule.

**Table 19.3** Trapezoid Rule for Various Step Sizes

Step size ( $\Delta X$ )	Volume (L)
0.45	47.85094
0.09	43.13532
0.05	42.98842
0.01	42.92521
0.005	42.92324
0.001	42.92260

added together to obtain the final answer. The results (to seven significant figures) for various step sizes are listed in Table 19.3. ■

### ILLUSTRATIVE EXAMPLE 19.4

The concentration,  $C$ , variation with length,  $z$ , in a 3 ft continuous contact mass transfer device is described by the equation:

$$\frac{dC}{C} = -\frac{k}{v} dz$$

where  $k$  is  $50 \text{ h}^{-1}$ ,  $v$  is  $50 \text{ ft/h}$ ,  $C$  is in  $\text{lbmol/ft}^3$ ,  $z$  is in feet and  $C = 1.0 \text{ lbmol/ft}^3$  at  $z = 0$ .

It has been proposed to represent the above with 10 staged units 0.3 ft in length. Develop solutions to this problem using a finite difference method of solving an ordinary differential equation and a lumped parameter model employing a method of solution of simultaneous linear algebraic equations.

#### SOLUTION:

##### *Finite Difference Method*

A finite difference procedure is now applied to the equation. The first derivative of  $C$  with respect to  $z$  is equivalent to the finite difference in the  $z$ -direction, i.e.,

$$\frac{dC}{dz} = \frac{\Delta C}{\Delta z} = \frac{C_{n+1} - C_n}{\Delta z}$$

Inserting this into the describing equation and noting that the average concentration over the increment should be used leads to

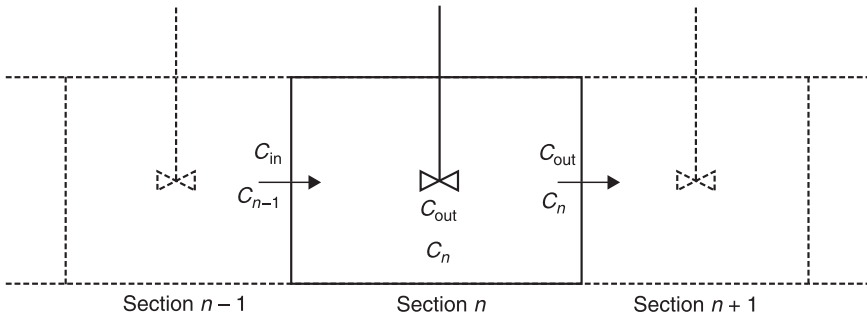
$$\frac{C_{n+1} - C_n}{\Delta z} = -\left(\frac{k}{v_z}\right) C_{\text{av}}$$

Knowing the initial condition, each successive concentration may be found by rearranging the above equation:

$$C_{n+1} = -\left(\frac{k\Delta z}{v_z}\right) C_{\text{av}} + C_n$$

The application of this equation requires a trial-and-error procedure where the average concentration over the increment is approximated and then checked when  $C_{n+1}$  is





**Figure 19.2** Lumped-parameter method.

calculated. One should note that the approximation part of this problem can be removed by replacing  $C_{av}$  by

$$\frac{C_{n+1} + C_n}{2}$$

and solving for  $C_{n+1}$  directly in terms of  $C_n$ .

### ***Lumped-parameter method***

In the lumped-parameter method, the device is divided into equal stages and each segment is considered to be a perfectly mixed vessel. This is shown schematically in Figure 19.2. The equation is now written as

$$\frac{C_{out} - C_{in}}{\Delta z} = -\frac{k}{v_z} C_{out}$$

Rearranging the above equation gives

$$C_{out} = \frac{C_{in}}{1 + \frac{k\Delta z}{v_z}}$$

If the initial concentration is  $C_0$  and the term

$$1 + \frac{k\Delta z}{v_z} = R$$

then the following set of equations are generated for each stage:

$$\begin{aligned} C_1 - RC_0 &= 0; && \text{first stage} \\ C_2 - RC_1 &= 0; && \text{second stage} \end{aligned}$$

⋮

$$C_{\text{final}} - RC_{\text{final}-1} = 0; \quad \text{final stage}$$

The above represents a series of (simultaneous) linear algebraic equations. These equations can be solved by a direct step-by-step hand calculation. Alternatively, a Gauss–Jordan or Gauss–Seidel method can also be used.

The results of the analyses by the two methods are combined and presented in tabular form for comparison along with the analytical solution (see Table 19.4). ■

**Table 19.4** Concentration Profile via Three Methods

$z$ , ft	Analytical	Finite-difference	Lumped-parameter
0.0	1.0000	1.0000	1.0000
0.3	0.8354	0.8358	0.8474
0.6	0.6980	0.7001	0.7181
0.9	0.5830	0.5863	0.6086
1.2	0.4870	0.4910	0.5157
1.5	0.4070	0.4112	0.4371
1.8	0.3400	0.3444	0.3704
2.1	0.2840	0.2884	0.3139
2.4	0.2370	0.2415	0.2660
2.7	0.1980	0.2022	0.2254

**ILLUSTRATIVE EXAMPLE 19.5**

The equation describing the concentration of a pollutant in a flowing river is given by

$$\frac{dC}{dt} = -0.580C + 6 \times 10^{-5}$$

with  $C_0 = 5.0 \times 10^{-5}$  gmol/cm<sup>3</sup> at  $t = 0$  min. Estimate  $C$  in gmol/cm<sup>3</sup> at 1 and 5 minutes. Use the Runge–Kutta method of analysis.<sup>(8)</sup>

**SOLUTION:** The Runge–Kutta (R–K) method is one of the most widely used techniques for solving first-order differential equations. For the equation

$$\frac{dy}{dx} = f(x, y) \quad (19.11)$$

the solution takes the form

$$y_{n+1} = y_n + \frac{h}{6}(D_1 + 2D_2 + 2D_3 + D_4) \quad (19.12)$$

where  $D_1 = hf(x, y)$

$$D_2 = hf\left(x_n + \frac{h}{2}, y_n + \frac{D_1}{2}\right)$$

$$D_3 = hf\left(x_n + \frac{h}{2}, y_n + \frac{D_2}{2}\right)$$

$$D_4 = hf(x_n + h, y_n + D_3)$$

The term  $h$  represents the increment in  $x$ . The term  $y_n$  is the solution to the equation at  $x_n$ , and  $y_{n+1}$  is the solution to the equation at  $x_{n+1}$  where  $x_{n+1} = x_n + h$ . Thus, the R–K method provides a straightforward means for developing expressions for  $\Delta y$  in terms of the function  $f(x, y)$  at various “locations” along the interval in question.

For a simple equation of the form

$$\frac{dC}{dt} = a + bC \quad (19.13)$$

where at  $t = 0$ ,  $C = C_0$ , the R–K algorithm given above becomes (for  $t = h$ )

$$C_1 = C_0 + \frac{h}{6}(D_1 + 2D_2 + 2D_3 + D_4) \quad (19.14)$$

where  $D_1 = hf(x, y) = h(a + bC_0)$

$$D_2 = hf\left(x_n + \frac{h}{2}, y_n + \frac{D_1}{2}\right) = h[a + b(C_0 + D_1/2)]$$

$$D_3 = hf\left(x_n + \frac{h}{2}, y_n + \frac{D_2}{2}\right) = h[a + b(C_0 + D_2/2)]$$

$$D_4 = hf(x_n + h, y_n + D_3) = h[a + b(C_0 + D_3)]$$

The same procedure is repeated to obtain values for  $C_2$  at  $t = 2h$ ,  $C_3$  at  $t = 3h$ , and so on.

Based on the data provided, evaluate the R–K coefficients for  $t = h$ :

$$D_1 = 1.0(6.0 - 2.9) = 3.1$$

$$D_2 = 1.0[6.0 - 0.58(5.0 + 3.1/2)] = 2.2$$

$$D_3 = 1.0[6.0 - 0.58(5.0 + 2.2/2)] = 2.46$$

$$D_4 = 1.0[6.0 - 0.58(5.0 + 2.46)] = 1.67$$

Calculate  $C_1$ :

$$\begin{aligned} C_1 &= C_0 + \frac{h}{6}(D_1 + 2D_2 + 2D_3 + D_4) \\ &= 5.0 + \frac{1}{6}[3.1 + 2(2.2) + 2(2.46) + 1.67] \\ &= 7.35 \text{ gmol/cm}^3 \end{aligned}$$

To calculate  $C_2$ :

$$D_1 = 1.0[6.0 - 0.58(7.35)] = 1.74$$

$$D_2 = 1.24$$

$$D_3 = 1.38$$

$$D_4 = 0.94$$

and

$$\begin{aligned} C_1 &= C_0 + \frac{h}{6}(D_1 + 2D_2 + 2D_3 + D_4) \\ &= 7.34 + \frac{1}{6}[1.74 + 2(1.24) + 2(1.38) + 0.94] \\ &= 8.66 \text{ gmol/cm}^3 \end{aligned}$$

Also calculate  $C_3$ ,  $C_4$ , and  $C_5$ :

$$\begin{aligned} C_3 &= 9.40 & \text{at } t = 3 \text{ min} \\ C_4 &= 9.81 & \text{at } t = 4 \text{ min} \\ C_5 &= 10.04 & \text{at } t = 5 \text{ min} \end{aligned}$$

The reader is left the exercise of comparing the numerical solution above (including that at  $t = \infty$ ) with that provided by the analytical solution.

The R–K method can also be used if the function also contains the independent variable. Consider the following equation:

$$\frac{dC}{dt} = f_1(C, t) \quad (19.15)$$

For this situation,

$$C_1 = C_0 + \frac{1}{6}(D_1 + 2D_2 + 2D_3 + D_4) \quad (19.16)$$

with

$$\begin{aligned} D_1 &= hf(C, t) \\ D_2 &= hf\left(C_0 + \frac{D_1}{2}, t_0 + \frac{h}{2}\right) \\ D_3 &= hf\left(C_0 + \frac{D_2}{2}, t_0 + \frac{h}{2}\right) \\ D_4 &= hf(C_0 + D_3, t_0 + h) \end{aligned}$$

If, for example,

$$\frac{dC}{dt} = 10C - e^{-ct}$$

then

$$D_2 = h \left[ 10 \left( C_0 + \frac{D_1}{2} \right) - e^{-[C_0 + (D_1/2)][t_0 + (h/2)]} \right]$$

Situations may arise when there is a need to simultaneously solve more than one ordinary differential equation (ODE). In a more general case, one could have  $n$  dependent variables  $y_1, y_2, \dots, y_n$ , with each related to a single independent variable  $x$  by the following system of  $n$  simultaneous first-order ODEs:

$$\begin{aligned} \frac{dy_1}{dx} &= f_1(x, y_1, y_2, \dots, y_n), \\ \frac{dy_2}{dx} &= f_2(x, y_1, y_2, \dots, y_n), \\ &\vdots \\ \frac{dy_n}{dx} &= f_n(x, y_1, y_2, \dots, y_n), \end{aligned} \quad (19.17)$$

Note that the equations in Equation (19.17) are interrelated, i.e., they are dependent on each other. This is illustrated in the following development.

Consider the following two equations:

$$\begin{aligned}\frac{dC}{dt} &= -Ae^{-ET/R}C = f(C, t) \\ \frac{dT}{dt} &= -kC \frac{\Delta H}{\rho C_P} = g(C, t)\end{aligned}\tag{19.18}$$

or, in a more general sense,

$$\begin{aligned}\frac{dy}{dx} &= f(x, y, z); \quad (\text{e.g., } xyz) \\ \frac{dz}{dt} &= g(x, y, z); \quad (\text{e.g., } x^2y^2e^{-z})\end{aligned}\tag{19.19}$$

The R–K algorithm for Equation (19.19) is

$$\begin{aligned}y_1 &= y_0 + \frac{1}{6}(RY_1 + 2RY_2 + 2RY_3 + RY_4) \\ z_1 &= z_0 + \frac{1}{6}(RZ_1 + 2RZ_2 + 2RZ_3 + RZ_4)\end{aligned}\tag{19.20}$$

where  $y_1 - y_0 = \Delta y$ ,  $z_1 - z_0 = \Delta z$ ,  $h = \Delta x$  and

$$\begin{aligned}RY_1 &= h \times f(x_0, y_0, z_0) \\ RZ_1 &= h \times g(x_0, y_0, z_0) \\ RY_2 &= h \times f(x_0 + h/2, y_0 + RY_1/2, z_0 + RZ_1/2) \\ RZ_2 &= h \times g(x_0 + h/2, y_0 + RY_1/2, z_0 + RZ_1/2) \\ RY_3 &= h \times f(x_0 + h/2, y_0 + RY_2/2, z_0 + RZ_2/2) \\ RZ_3 &= h \times g(x_0 + h/2, y_0 + RY_2/2, z_0 + RZ_2/2) \\ RY_4 &= h \times f(x_0 + h, y_0 + RY_3, z_0 + RZ_3) \\ RZ_4 &= h \times g(x_0 + h, y_0 + RY_3, z_0 + RZ_3)\end{aligned}$$

Although the R–K approach (and other companion methods) have traditionally been employed to solve first-order ODEs, it can also treat higher ODEs. The procedure requires reducing an  $n$ th order ODE to a first-order ODE. For example, if the equation is of the form<sup>(9)</sup>

$$\frac{d^2y}{dx^2} = f(y, x)\tag{19.21}$$

set

$$z = \frac{dy}{dx}\tag{19.22}$$

so that

$$\frac{dz}{dx} = \frac{d^2y}{dx^2}\tag{19.23}$$

The second-order equation in Equation (19.21) has now been reduced to the two first-order ODEs in Equation (19.24):

$$\begin{aligned}\frac{d^2y}{dx^2} &= \frac{dz}{dx} = f(y, x) \\ \frac{dy}{dx} &= z\end{aligned}\tag{19.24}$$

The procedure set forth in Equations (19.19) and (19.20) can be applied to generate a solution to Equation (19.21). Note, however, that the first derivative (i.e.,  $dy/dx$  or its estimate) is required at the start of the integration. Extending the procedure to higher-order equations is left as an exercise for the reader. ■

### ILLUSTRATIVE EXAMPLE 19.6

The vapor pressure,  $p'$ , for a new synthetic chemical at a given temperature has been determined to take the form:

$$p' = T^3 - 2T^2 + 2T$$

If  $p' = 1$ , one may then write

$$f(T) = T^3 - 2T^2 + 2T - 1 = 0$$

where the term  $T$  is in K. The actual temperature,  $t$ , is given by

$$t = 10^3 T$$

Solve the above equation for the actual temperature in K for  $p' = 1.0$ . Earlier studies indicate that  $t$  is in the 1000–1200 K range.

**SOLUTION:** The subject of the solution to a nonlinear algebraic equation is considered in this example. Although several algorithms are available, the presentation will key on the Newton–Raphson method of evaluating the root(s) of a nonlinear algebraic equation.

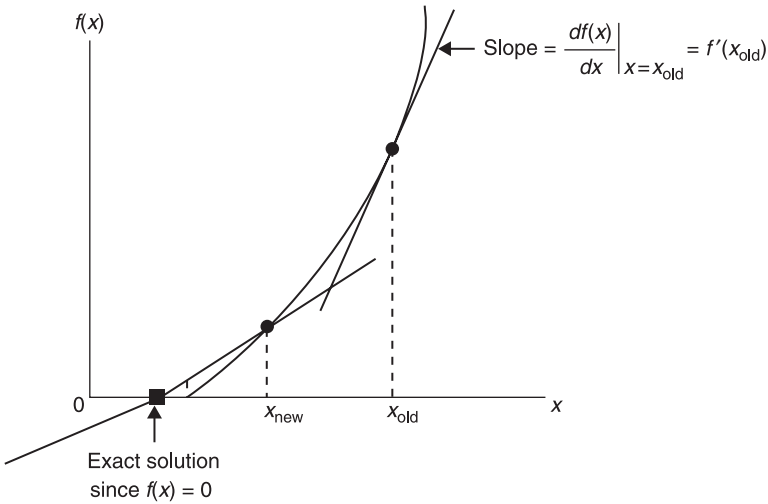
The solution to the equation

$$f(x) = 0\tag{19.25}$$

is obtained by guessing a value for  $x$  ( $x_{\text{old}}$ ) that will satisfy the above equation. This value is continuously updated ( $x_{\text{new}}$ ) using the recursion equation

$$x_{\text{new}} = x_{\text{old}} - \frac{f(x_{\text{old}})}{f'(x_{\text{new}})}\tag{19.26}$$

until either little or no change in  $(x_{\text{new}} - x_{\text{old}})/x_{\text{old}}$  is obtained. One can express this operation graphically (see Fig. 19.3).



**Figure 19.3** Newton–Raphson method.

Noting that

$$f'(x_{\text{old}}) = \frac{df(x)}{dx} \approx \frac{\Delta f(x)}{\Delta x} = \frac{f(x_{\text{old}}) - 0}{x_{\text{old}} - x_{\text{new}}} \quad (19.27)$$

one may rearrange Equation (19.27) to yield Equation (19.26). The  $x_{\text{new}}$  then becomes the  $x_{\text{old}}$  in the next calculation.

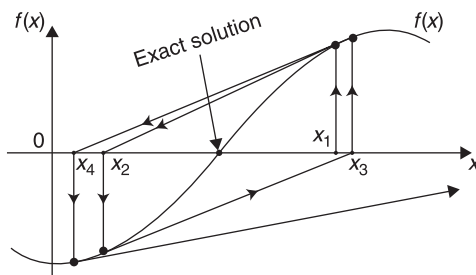
This method is also referred to as Newton's method of tangents and is a widely used method for improving a first approximation to a root to the aforementioned equation of the form  $f(x) = 0$ . The above development can be rewritten in subscripted form to accommodate a computer calculation. Thus,

$$f'(x_n) = \frac{f(x_n)}{x_n - x_{n+1}} \quad (19.28)$$

from which

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)} \quad (19.29)$$

where  $x_{n+1}$  is again the improved estimate of  $x_n$  and the solution to the equation  $f(x) = 0$ . For this procedure, the value of the function and the value of the derivative of the function are determined at  $x = x_n$ , and the new approximation to the root,  $x_{n+1}$ , is obtained. The same procedure is repeated, with the new approximation, to obtain a still better approximation of the root. This continues until successive values for the approximate root differ by less than a prescribed small value,  $\varepsilon$ , which controls the allowable error (or tolerance) in the root. Relative to the previous



**Figure 19.4** Failure of the Newton–Raphson method.

estimate,

$$\varepsilon = \frac{x_{n+1} - x_n}{x_n} \quad (19.30)$$

Despite its popularity, the method suffers for two reasons. First, an analytical expression for the derivative [i.e.,  $f'(x_n)$ ] is required. In addition to the problem of having to compute an analytical derivative value at each iteration, one would expect Newton's method to converge fairly rapidly to a root in the majority of cases. However, as is common with most numerical methods, it may fail occasionally. A possible initial oscillation followed by a displacement away from a root is illustrated in Figure 19.4. Note, however, that the method would have converged (in this case) if the initial guess had been somewhat closer to the exact root. Thus, it can be seen that the initial guess may be critical to the success of the calculation.

With reference to the problem, assume an initial temperature  $t_1$ . Set  $t_1 = 1100$  so that

$$T_1 = (1100)(10^{-3}) = 1.1$$

Obtain the analytical derivative,  $f'(T)$ :

$$f'(T) = 3T^2 - 4T + 2$$

Calculate  $f(T_1)$  and  $f'(T_1)$ :

$$f(1.1) = T^3 - 2T^2 + 2T - 1 = (1.1)^3 - 2(1.1)^2 + 2(1.1) - 1 = 0.111$$

$$f'(1.1) = 3T^2 - 4T + 2 = 3(1.1)^2 - 4(1.1) + 2 = 1.23$$

Use the Newton–Raphson method to estimate  $T_2$ . Employ Equation (19.26):

$$T_2 = T_1 - \frac{f(T_1)}{f'(T_1)} = 1.1 - \frac{0.111}{1.23} = 1.0098$$

Calculate  $T_3$ :

$$f(T_2) = 0.0099$$

$$f'(T_2) = 1.0198$$

$$T_3 = 1.0001$$

Finally, calculate the best estimate (based on two iterations) of  $t$ :

$$t = 1000.1 \text{ K}$$



Other methods that may be employed include:

- 1 Wegstein's method
- 2 False-position
- 3 Half-interval
- 4 Second-order Newton–Raphson

Details are available in the literature.<sup>(2,3)</sup> ■

### ILLUSTRATIVE EXAMPLE 19.7

Qualitatively discuss methods of solving partial differential equations.

**SOLUTION:** Many practical problems in engineering involve at least two independent variables, i.e., the dependent variable is defined in terms of (or is a function of) more than one independent variable. The derivatives describing these independent variables are defined as partial derivatives. Differential equations containing partial derivatives are referred to as partial differential equations (PDEs).

Contrary to a widely accepted myth, an engineer's mathematical obligations do not end after formulating an equation for a problem, where it may be given to a mathematician to solve. Even if such an ideal situation should exist, it is still necessary for engineers to have a reasonable understanding of the mathematical methods and their limitations employed in the solution in order to interpret results.

It has been said that “the solution of a partial differential equation is essentially a guessing game.” In other words, one cannot expect to be given a formal method that will yield exact solutions for all partial differential equations.<sup>(8)</sup> Fortunately, numerical methods for solving these equations were developed during the middle and latter part of the 20th century.

The three main PDEs encountered in engineering practice are briefly introduced below employing  $C$  (e.g., the concentration as the independent variable).

The parabolic equation:

$$\frac{\partial C}{\partial t} = \frac{\partial^2 C}{\partial x^2} \quad (19.31)$$

The elliptical equation:

$$\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} = 0 \quad (19.32)$$

The hyperbolic equation:

$$\frac{\partial^2 C}{\partial t^2} = \frac{\partial^2 C}{\partial x^2} \quad (19.33)$$

The preferred numerical method of solution involves finite differencing. Only the parabolic and elliptical equations are considered below. Examples of parabolic PDEs include

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \quad (19.34)$$

and (the two-dimensional)

$$\frac{\partial C}{\partial t} = D \left[ \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} \right] \quad (19.35)$$

Ketter and Prawel,<sup>(3)</sup> as well as many others, have reviewed the finite difference approach to solving Equation (19.34). ■

### ILLUSTRATIVE EXAMPLE 19.8

Qualitatively discuss optimization.

**SOLUTION:** Optimization is viewed by many as a tool in decision-making. It often aids in the selection of values that allow the practicing engineering to better solve a problem. This brief answer provides a qualitative look at optimization.

In its most elementary and basic form, one may say that optimization is concerned with the determination of the “best” solution to a given problem. This process is required in the solution of many general problems in engineering and applied science—in the maximization (or minimization) of a given function(s), in the selection of a control variable to facilitate the realization of a desired condition, in the scheduling of a series of operations or events to control completion dates of a given project, in the development of optimal layouts of organizational units within a given design space, etc.<sup>(4)</sup>

The optimization problem has been described succinctly by Aris<sup>(10)</sup> as “getting the best you can out of a given situation.” Problems amenable to solution by mathematical optimization techniques have the general characteristics that

- 1 there are one or more independent variables whose values must be chosen to yield a viable solution, and
- 2 there is some measure of “goodness” available to distinguish between the many viable solutions generated by different choices of these variables.

Mathematical optimization techniques are used for guiding the problem solver to that choice of variables that maximizes the goodness measure (profit, for example) or that minimizes some badness measure (cost, for example).

One of the most important areas for the application of mathematical optimization techniques is in engineering design. Applications include:

- 1 the generation of “best” functional representations (curve fitting, for example),
- 2 the design of optimal control systems,
- 3 determining the optimal height (or length) of a mass transfer unit,
- 4 determining the optimal diameter of a unit,
- 5 finding the best equipment materials of construction,
- 6 generating operating schedules, and
- 7 selecting operating conditions.

Once a particular subject or process scheme has been selected for study, it is common practice to optimize the process from a capital cost and O&M (operation and maintenance) standpoint.

There are many optimization procedures available, most of them too detailed for meaningful application in a text of this nature. These sophisticated optimization techniques, some of which are routinely used in the design of conventional chemical and petrochemical plants, invariably involve computer calculations. However, use of these techniques in the majority of industrial applications is not warranted.<sup>(11)</sup> ■

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