

# Chapter 26

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## Numerical Methods

### INTRODUCTION

Chapter 26 is concerned with Numerical Methods. This subject was taught in the past as a means of providing engineers and scientists with ways to solve complicated mathematical expressions that they could not solve otherwise. However, with the advent of computers, these solutions have become readily obtainable.

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 author has not attempted to cover all the topics of Numerical Methods. There are several excellent texts in the literature that deal with this subject matter in more detail.<sup>(1,2)</sup>

Ordinarily, discussion of the following eight numerical methods would be included in this chapter:

1. Simultaneous linear algebraic equations.
2. Nonlinear algebraic equations.
3. Numerical integration.
4. Numerical differentiation.
5. Ordinary differential equations.
6. Partial differential equations, including Monte Carlo methods.
7. Regression analysis.
8. Optimization.

However, because of the breadth of the subject matter, the reader should note that only the last three numerical methods receive treatment in the chapter. The remaining five methods are to be found in the literature.<sup>(3,4)</sup> It should be noted that the Applications Section contains heat transfer material dealing with the later three topics.

## HISTORY

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. The reader should note that one rarely needs exact answers in technical practice. Most real-world solutions 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, often representing a system or process, exact solutions may not be attainable. 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 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 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>(5)</sup>

One of the earliest modern day computers (perhaps more appropriately called a calculator) appeared on the scene in 1914. A new patented indicator or runner for slide rules, called the “frameless,” was perfected by Keuffel & Esser Co. The “framless” was unique in that every figure on the rule was clearly visible at all times such there was no side piece(s) to the metal holder of the glass indicator. In 1968, Hewlett-Packard announced the development of a calculator that could “deftly handle arithmetically large numbers”; the calculator weighted 40 lbs and cost nearly \$5000.

A procedure-oriented language (POL) is a way of expressing commands to a computer in a form somewhat similar to such natural languages as English and mathematics. The instructions that make up a program written in a POL are called the source code. Because the computer understands only machine language (or object code), a translator program must be run to translate the source code into an object code. In terms of input, processing, and output, the source code is the input to the translator program, which processes (translates) the code. The output is the object code. It is the object code that is actually executed in order to process data and information.

The first POL to be widely used was FORTRAN, an acronym that was coined from the words “FORMula TRANslation.” FORTRAN was designed initially for use on problems of a mathematical nature and it is still used for solving some problems in mathematics, engineering, and science.

PASCAL is a POL designed by Niklaus Wirth in 1968. The motivation behind its design was to provide a language that encouraged the programmer to write programs according to the principles of structured programming. An important aspect of the PASCAL design philosophy is that it is a “small” language. The purpose of this is to provide the programmer with a language that can be easily learned and retained. PASCAL is also most commonly used in mathematics, engineering and science.

BASIC is an acronym for Beginner’s All-purpose Symbolic Instruction Code. J. G. Kemeny and T. E. Kurtz developed BASIC in 1967 to give students a simple language for learning programming. BASIC is an interactive language; i.e., the programmer sees an error or output as soon as it occurs. The simplicity of BASIC makes it easy to learn and use. Many versions of BASIC have been written since the late 1960s. BASIC can be used effectively for a variety of business and scientific applications.

Two types of translator programs—compilers and interpreters—are used to convert program statements to a machine-readable format. A compiler first translates the entire program to machine language. If any syntax or translation errors are encountered, a complete listing of each error and the incorrect statement is given to the programmer. After the programmer corrects the errors, the program is compiled again. When no errors are detected, the compiled code (object code) can be executed. The machine-language version can then be saved separately so that the compiling step need not be repeated each time the program is executed unless the original program is changed. Compiled programs run much faster than the interpreted ones. An interpreter translates and executes one source code instruction of a program at a time. Each time an instruction is executed, the interpreter uses the key words in the source code to call pre-written machine-language routines that perform the functions specified in the source code. The disadvantage of an interpreter is that the program must be translated each time it is executed.

The general availability of computers has been followed by a near infinite number of application programs, promising relief from the aforementioned slide rule. Many of these programs deal with design optimization for heat exchangers as well as other process equipment and full scale plant applications. Today, many powerful commercial mathematical applications are available and widely used in academia and industry. Some of these programs include MathCad, Matlab, Mathematica, etc. These user-friendly programs allow engineers and scientists to perform mathematical calculations without knowing any programming. In addition, new programs, for example, Visual Basic, .NET, JAVA, C++, etc., are constantly evolving. These software packages are the modern day slide rule for the 21st century engineer and the numerical methods listed below provide the “instructions” on how to properly use this new slide rule.

With commercial mathematical application’s powerful computing ability, learning the numerical procedures involved does little for the practicing engineer in terms of interpreting and analyzing answers. For example, instead of performing a numerical

integration using the trapezoid rule, one can use one of the programs mentioned above to do the calculation. However, the job of the engineer then becomes that of assessing if the answer given by the computer program seems reasonable. If it does, one can be fairly certain the numbers are correct (providing the rest of the input was correct), but if the answer seems unreasonable, the engineer's job is to figure out what technique the program is using and what might cause it to return an incorrect answer (or, more precisely, a correct answer to the equation, but not to the problem).

## PARTIAL DIFFERENTIAL EQUATIONS

Many practical problems in engineering involve at least two independent variables; that is, 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 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 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>(6)</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  $T$  (e.g., the temperature as the dependent variable) with  $t$  (time) and  $x, y, z$  (position) the independent variables.

The parabolic equation:

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial z^2} \quad (26.1)$$

The elliptical equation:

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0 \quad (26.2)$$

The hyperbolic equation:

$$\frac{\partial^2 T}{\partial t^2} = \alpha \frac{\partial^2 T}{\partial x^2} \quad (26.3)$$

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

### Parabolic PDE

Examples of parabolic PDEs include

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \tag{26.4}$$

and (the two-dimensional)

$$\frac{\partial T}{\partial t} = \alpha \left[ \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right] \tag{26.5}$$

Ketter and Prawler,<sup>(2)</sup> as well as many others, have reviewed the finite difference approach to solving Equation (26.4). This is detailed below.

Consider the  $(t, x)$  grid provided in Figure 26.1. The partial derivatives may be replaced by

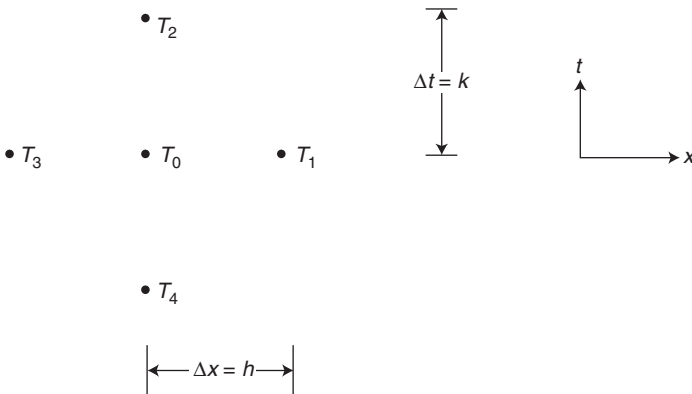
$$\frac{\partial T}{\partial t} \cong \frac{\Delta T}{\Delta t} = \frac{-T_4 + T_2}{2(\Delta t)} = \frac{-T_4 + T_2}{2k}; \Delta t = k \tag{26.6}$$

and

$$\frac{\partial^2 T}{\partial x^2} \cong \frac{\Delta}{\Delta x} \left( \frac{\Delta T}{\Delta x} \right) = \frac{T_3 - 2T_0 - T_1}{h^2}; \Delta x = h \tag{26.7}$$

Substituting Equations (26.6) and (26.7) into Equation (26.4) leads to

$$\frac{-T_4 - T_2}{2k} = \frac{T_3 - 2T_0 - T_1}{h^2} \tag{26.8}$$



**Figure 26.1** Parabolic grid.

Solving for  $T_2$ :

$$T_2 = T_4 + 2r(T_3 - 2T_0 - T_1) \quad (26.9)$$

where  $r = k/h^2$ ,

Thus,  $T_2$  may be calculated if  $T_0$ ,  $T_1$ ,  $T_3$ , and  $T_4$  are known. Unfortunately, stability and error problems arise employing the above approach. These can be removed by replacing the central difference term in Equation (26.6) by a forward difference term, that is,

$$\frac{\partial T}{\partial t} \cong \frac{\Delta T}{\Delta t} = \frac{-T_0 + T_2}{(\Delta t)} = \frac{-T_0 + T_2}{k} \quad (26.10)$$

With this substitution, Equation (26.9) becomes

$$T_2 = T_0 + r(T_3 - 2T_0 + T_1) \quad (26.11)$$

It can be shown that the problem associated with the central difference derivative is removed if  $r \leq 0.5$ .

An unsteady-state heat conduction experiment conducted at Manhattan College's Unit operations laboratory is concerned with the application of this equation. In the experiment, a 316 stainless steel rod is heated at each end with steam at temperature  $T_S$ . The initial temperature of the rod is  $T_A$ . The describing equation and Ba/o IC(s) for this system are

$$\frac{\partial T}{\partial t} = \alpha \frac{\partial^2 T}{\partial x^2} \quad (26.1)$$

$$\text{BC(1): } T = T_S \text{ at } x = 0$$

$$\text{BC(2): } T = T_S \text{ at } x = L$$

$$\text{IC: } T = T_A \text{ at } t = 0, 0 \leq x \leq L$$

The solution to this equation can be shown<sup>(7)</sup> to be:

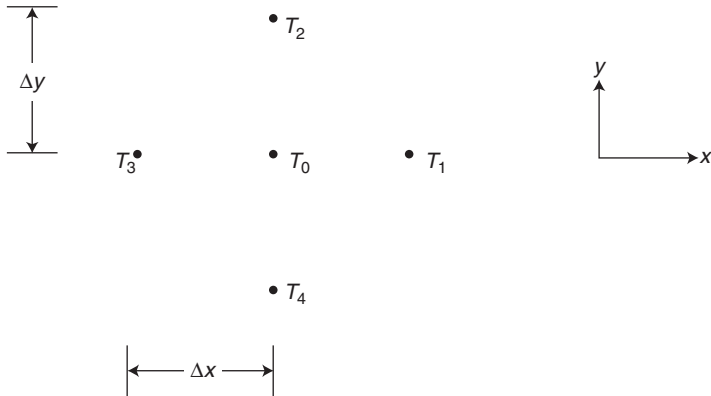
$$T = T_S + (T_A - T_S) \left\{ \sum_{n=1}^{\infty} 2 \left[ \frac{(-1)^{n+1} + 1}{n\pi} \right] e^{-\alpha(n\pi/2)^2 t} \sin\left(\frac{n\pi x}{2}\right) \right\} \quad (26.12)$$

The reader may choose to (again) review this essentially same problem in Illustrative Example 8.3.

## Elliptical PDE

For this equation, examine the grid in Figure 26.2. Using finite differences in Equation (26.2) ultimately leads to

$$T_0 = \frac{1}{4}(T_1 + T_2 + T_3 + T_4); \Delta x = \Delta y \quad (26.13)$$

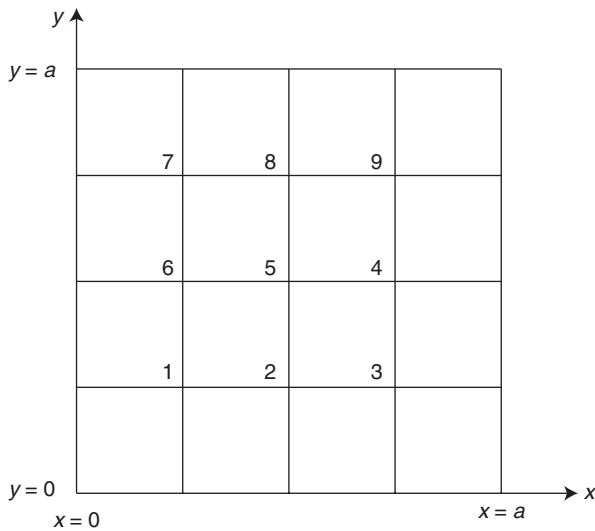


**Figure 26.2** Elliptic grid.

In effect, each  $T$  value reduces to the average of its four nearest neighbors in the square grid. This difference equation may then be written at each interior grid point, resulting in a linear system of  $N$  equations, where  $N$  is the number of grid points. The system can then be solved by one of several methods provided in the literature.<sup>(1,2,7)</sup>

Another method of solution involves applying the Monte Carlo approach, requiring the use of random numbers.<sup>(7)</sup> Considered the square pictured in Figure 26.3. If the describing equation for the variation of  $T$  within the grid structure is

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0 \tag{26.14}$$



**Figure 26.3** Monte Carlo grid.

with specified boundary conditions (BC) for  $T(x, y)$  of  $T(0, y)$ ,  $T(a, y)$ ,  $T(x, 0)$ , and  $T(x, a)$  one may employ the following approach.

1. Proceed to calculate  $T$  at point 1 (i.e.,  $T_1$ ).
2. Generate a random number between 00 and 99.
3. If the number is between 00–24, move to the left. For 25–49, 50–74, 75–99, move upward, to the right, and downward, respectively.
4. If the move in step 3 results in a new position that is at the outer surface (boundary), terminate the first calculation for point 1 and record the  $T$  value of the boundary at the new position. However, if the move results in a new position that is not at a boundary, and is still at one of the other eight interval grid points, repeat steps (2) and (3). This process is continued until an outer surface or boundary is reached.
5. Repeat steps (2–4) numerous times, e.g., 1000 times.
6. After completing step (5), sum all the  $T$  values obtained and divided this value by the number of times steps (2–4) have been repeated. The resulting value provides a reasonable estimate of  $T_1$ .
7. Return to step (1) and repeat the calculation for the remaining eight grid points.

This method of solution is not limited to square systems. The general energy equation for heat transfer in solids is once again presented below for rectangular, cylindrical, and spherical coordinate systems. See also Chapters 7 and 8.

Rectangular coordinates:

$$\frac{\partial T}{\partial t} = \alpha \left[ \frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right] \quad (26.15)$$

Cylindrical coordinates:

$$\frac{\partial T}{\partial t} = \alpha \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 T}{\partial \phi^2} + \frac{\partial^2 T}{\partial z^2} \right] \quad (26.16)$$

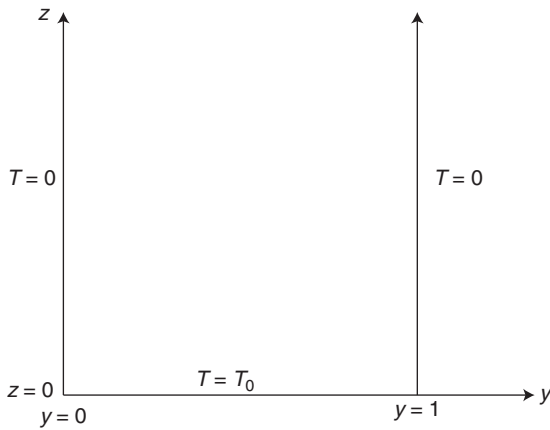
Spherical coordinates:

$$\frac{\partial T}{\partial t} = \alpha \left[ \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial T}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial T}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 T}{\partial \phi^2} \right] \quad (26.17)$$

### ILLUSTRATIVE EXAMPLE 26.1<sup>(8)</sup>

Consider the two-dimensional problem of a very thin solid bounded by the  $y$ -axis ( $z = 0$ ), the lines  $y = 0$  and  $y = 1$ , and extending to infinity in the  $z$ -direction. The temperature  $T$  of the





**Figure 26.4** System in Illustrative Example 26.1.

vertical edge at  $y = 0$  and  $y = 1$  is maintained at zero.  $T$  at  $z = 0$  is  $T_0$ . Obtain the equation describing the steady-state profile of  $T$  in the solid. Refer to Figure 26.4.

**SOLUTION:** Select rectangular coordinates. Based on the problem statement,  $T$  is not a function of  $x$ . Thus,  $T$  is solely a function of  $y$  and  $z$ . Thus,  $T = T(y, z)$ . The following equation is extracted from Equation (26.15) provided above.

$$\frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} = 0$$

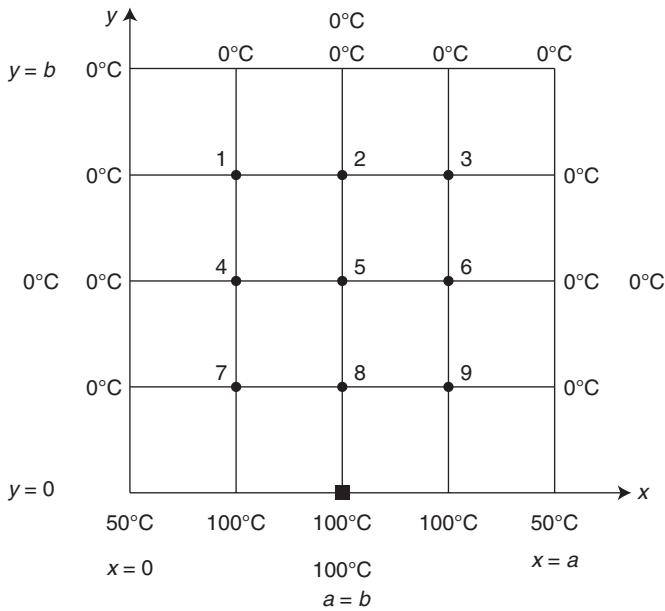
One can show that the analytical solution to the describing equation, subject to the boundary conditions specified is:<sup>(9)</sup>

$$T = \sum_{n=1}^{\infty} \frac{2T_0}{n\pi} [(-1)^{n+1} + 1] e^{-(n\pi/1)z} \sin\left(\frac{n\pi y}{1}\right)$$

■

### ILLUSTRATIVE EXAMPLE 26.2

Consider the system pictured in Figure 26.5. If the system is solid and the variable  $T$  is the temperature, the elliptical equation provided in Equation (26.2) applies. For this system, the temperature at each location is given by the average temperature of its four neighboring points. Using the Monte Carlo procedure provided earlier in this section and in Chapter 24 (see Illustrative Example 26.10 later), generate the temperature profile in the solid.



**Figure 26.5** Temperature grid for a square.

**SOLUTION:** Using the Monte Carlo algorithm provided and a random number generator leads to the following results

- $T_1 = 7.07^\circ\text{C}$
- $T_2 = 9.80^\circ\text{C}$
- $T_3 = 7.16^\circ\text{C}$
- $T_4 = 18.67^\circ\text{C}$
- $T_5 = 25.12^\circ\text{C}$
- $T_6 = 18.77^\circ\text{C}$
- $T_7 = 42.93^\circ\text{C}$
- $T_8 = 52.57^\circ\text{C}$
- $T_9 = 42.80^\circ\text{C}$



This procedure can be extended to rectangles; it is not limited to squares. If a rectangle is subjected to the following (somewhat similar) boundary conditions.

$$\begin{aligned}
 T(x = 0, \text{ any } y) &= T_0 \\
 T(x = b, \text{ any } y) &= 0 \\
 T(\text{any } x, y = +a) &= 0 \\
 T(\text{any } x, y = -a) &= 0
 \end{aligned}$$

The analytical solution for the above rectangle ( $2a$  by  $b$ ) is

$$T = 2T_0 \sum_{n=0}^{\infty} \left\{ \frac{(-1)^n}{\lambda_n a} \right\} \left\{ \frac{\sinh[\lambda_n(b-x)]}{\sinh(\lambda_n b)} \right\} \cos(\lambda_n y)$$

where  $\lambda_n = \frac{(2n+1)\pi}{2a}$ ;  $n = 0, 1, 2, 3 \dots$

### ILLUSTRATIVE EXAMPLE 26.3

Solve Illustrative Example 26.2 using the Gauss-Elimination method.

**SOLUTION:**<sup>(9)</sup> The familiar finite difference approach will be employed. For example,

$$T_5 \equiv (1/4)[T_2 + T_4 + T_6 + T_8]$$

This form of the equation may be applied to the nine points, which sets each  $T$  equal to the average of temperature of its four neighboring points. This produces a set of nine equations with nine unknowns. Employing Mathematica, Mathcad, Excel or a similar program leads to

$$\begin{aligned} T_1 &= 7.14^\circ\text{C} \\ T_2 &= 9.82^\circ\text{C} \\ T_3 &= 7.14^\circ\text{C} \\ T_4 &= 18.75^\circ\text{C} \\ T_5 &= 25^\circ\text{C} \\ T_6 &= 18.75^\circ\text{C} \\ T_7 &= 42.86^\circ\text{C} \\ T_8 &= 52.68^\circ\text{C} \\ T_9 &= 42.86^\circ\text{C} \end{aligned}$$

■

### ILLUSTRATIVE EXAMPLE 26.4

Comment on the results of the two previous examples.

**SOLUTION:** As expected the results are in reasonable agreement with each other. In addition,

$$T_8 > T_7 > T_5 > T_4 > T_2 > T_1$$

with,

$$T_1 \cong T_3$$

$$T_4 \cong T_6$$

$$T_7 \cong T_9$$

■

### ILLUSTRATIVE EXAMPLE 26.5

Outline how to solve the previous example if the face surface is a rectangle solid (see Figure 26.6).

**SOLUTION:** The outline of the calculation presented in the previous examples remains the same. ■

### ILLUSTRATIVE EXAMPLE 26.6

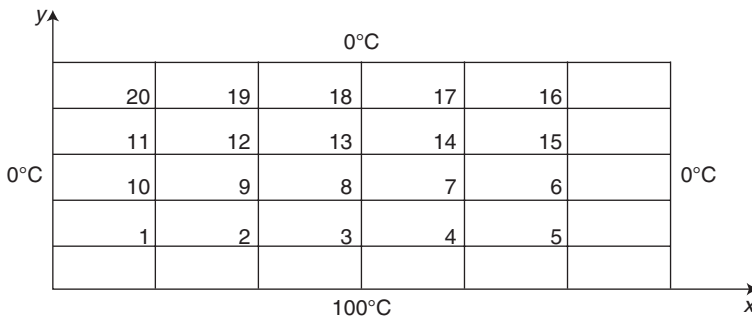
A rectangular walled stack (see Figure 26.7) serves as the discharge conduit for flue gases from an incinerator. If the inner and outer (atmosphere) steady-state temperatures are  $1700^\circ\text{F}$  and  $1400^\circ\text{F}$  respectively, calculate the temperature profile in the stack wall.

**SOLUTION:** Due to symmetric only the local temperatures in the bottom part of Figure 26.7, i.e., points (nodes) 4–12, will be calculated. First note, that

$$T_1 = T_2 = T_3 = T_4 = 1700^\circ\text{F}$$

$$T_{13} = T_{14} = T_{15} = T_{16} = T_{17} = T_{18} = 1400^\circ\text{F}$$

Neglecting “curvature” effects, one notes that the temperature at nodes below points 3 and 4 are approximately equal. Applying the appropriate equation at each node leads to 9 equations



**Figure 26.6** Rectangular grid; Illustrative Example 26.5.

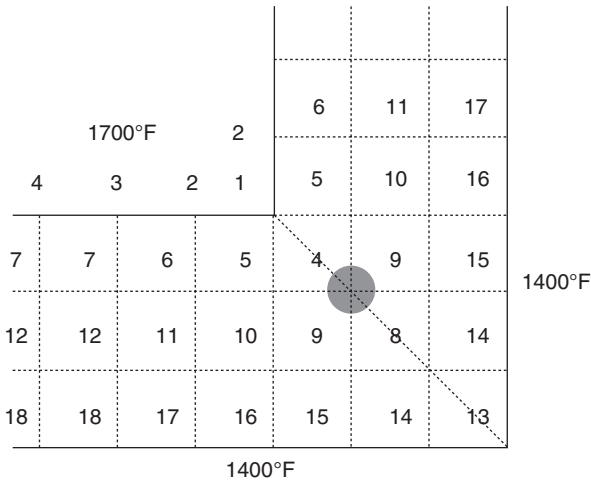


Figure 26.7 Stack temperature profile; Illustrative Example 26.6.

and 9 unknowns

$$\begin{aligned}
 4: \quad T_4 &= (2T_5 + 2T_9)/4 \\
 5: \quad T_5 &= (T_4 + T_6 + T_{10} + 1700)/4 \\
 6: \quad T_6 &= (T_5 + T_7 + T_{11} + 1700)/4 \\
 7: \quad T_7 &= (2T_6 + T_{12} + 1700)/4 \\
 8: \quad T_8 &= (2T_9 + 1400 + 1400)/4 \\
 9: \quad T_9 &= (T_4 + T_8 + T_{10} + 1400)/4 \\
 10: \quad T_{10} &= (T_5 + T_9 + T_{11} + 1400)/4 \\
 11: \quad T_{11} &= (T_6 + T_{10} + T_{12} + 1400)/4 \\
 12: \quad T_{12} &= (T_7 + 2T_{11} + 1400)/4
 \end{aligned}$$

Employing a suitable numerical method proposed in an earlier example leads to:

$$\begin{aligned}
 T_4 &= 312^\circ\text{F} & T_7 &= 392^\circ\text{F} & T_{10} &= 278^\circ\text{F} \\
 T_5 &= 370^\circ\text{F} & T_8 &= 227^\circ\text{F} & T_{11} &= 290^\circ\text{F} \\
 T_6 &= 388^\circ\text{F} & T_9 &= 254^\circ\text{F} & T_{12} &= 292^\circ\text{F}
 \end{aligned}$$



**ILLUSTRATIVE EXAMPLE 26.7**

Comment on the results of the previous illustrative example.

**SOLUTION:** The results are consistent. As one would expect

$$\begin{aligned}T_7 &> T_{12} \\T_6 &> T_{11} \\T_5 &> T_{10} \\T_4 &> T_9 > T_8\end{aligned}$$

In addition,

$$\begin{aligned}T_6 &\simeq T_7 \\T_{11} &\simeq T_{12}\end{aligned}$$

■

## REGRESSION ANALYSIS

The application of statistics in practice during the past several decades is so extensive that every practicing engineer should possess a basic knowledge of this branch of mathematics. In many applications, statistics enables one to obtain the most information out of his/her data. Although statistical methods are often a poor substitute for rigorous mathematical analyses, they frequently can be used where too little is known about a process or system to permit a rigorous mathematical treatment.

Regression analysis is a useful statistical technique for developing a quantitative relationship between a dependent variable and one or more independent variables. It usually utilizes experimental data on the pertinent variables to develop a numerical equation showing the influence of the independent variables on the dependent variable of the system. A simple correlation problem can arise when one asks whether there is any relationship between smoking and heart ailments, between beauty and brains, between pressure drop and velocity, between particle drag force and fluid density, etc. For example, in a tubular flow reactor involving a complex chemical reaction, regression methods have been used to develop an equation relating the yield of a desired product to entering concentrations, temperature, pressure, and residence time.<sup>(10)</sup>

Consider two random variables  $x$  and  $y$  and the problem of determining the extent to which they are related. The investigation of the relationship between two such variables, based on a set of  $n$  pairs of measurements  $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ , usually begins with an attempt to discover the approximate form of the relationship by graphing the data as  $n$  points in the  $x, y$ -plane. Such a graph is called a *scatter diagram*. Use of a scatter diagram allows one to quickly discern whether there is any pronounced relationship and, if so, whether the relationship may be treated as approximately linear.<sup>(11)</sup>

One of the problems of fitting a curve to a set of points in some efficient manner is essentially that of estimating the parameters of the curve in an efficient manner. Although there are numerous methods for performing the estimation of such parameters, the best known and most popular method is known as the method of least squares.

Since the desired equation is generally used for estimating or predicting purposes, it is reasonable to expect that it leads to small errors of estimation. An error of estimation or prediction is defined as the difference between an observed value of  $y$  and the corresponding fitted curve value of  $y$ . If the value of the variable to be estimated is denoted by  $y$  and the corresponding curve value by  $y'$ , then the error of estimation,  $E$ , is given by  $y - y'$ . Since the errors may be positive or negative and might add up to a small value for a poorly fitted curve, it will not do to merely require that the sum of the errors be as small as possible. This difficulty can be removed by requiring that the sum of the absolute values of the errors be as small as possible. However, sums of absolute values are not convenient to work with mathematically; consequently, the difficulty is avoided by requiring that the sum of the squares of the errors be minimized. The values of the parameters obtained by this minimization procedure determines what is known as the best fitting curve in the sense of least squares.<sup>(11)</sup>

The method of least squares is based on the assumption that the sum of the squares of the deviations between the assumed function and the given data, i.e., the sum of these errors, must be a minimum. If the ordinate of the data point is designated as  $y_i$  and the value of the approximating function at the same value of  $x_i$  is  $f(x_i)$ , the error at  $x_i$  can be written as

$$E_i = y_i - f(x_i) \quad (26.18)$$

Mathematically, the method of least squares requires that

$$\sum_{i=1}^n E_i^2 = \sum_{i=1}^n [y_i - f(x_i)]^2 = \text{minimum} \quad (26.19)$$

where  $n$  is the number of data points.

For illustration, assume a second-order polynomial, as given by Equation (26.20).

$$f(x) = a_0 + a_1x + a_2x^2 \quad (26.20)$$

The error,  $E_i$ , at each data point,  $i$ , is therefore

$$E_i = a_0 + a_1x + a_2x^2 - y_i \quad (26.21)$$

The sum of the errors squared,  $S$ , is

$$S = \sum E_i^2 = \sum (a_0 + a_1x + a_2x^2 - y_i)^2 \quad (26.22)$$

The requirement for this function,  $S$ , to be a minimum is given by

$$\left. \frac{\partial S}{\partial a_2} \right|_{a_1, a_0} = 0; \quad \left. \frac{\partial S}{\partial a_1} \right|_{a_2, a_0} = 0; \quad \left. \frac{\partial S}{\partial a_0} \right|_{a_2, a_1} = 0 \quad (26.23)$$

These three equations can be shown to reduce to<sup>(12)</sup> (for Equation (26.20))

$$\begin{aligned} \sum_{i=1}^n 2x_i^2(a_2x_i^2 + a_1x_i + a_0 - y_i) &= 0 \\ \sum_{i=1}^n 2x_i(a_2x_i^2 + a_1x_i + a_0 - y_i) &= 0 \\ \sum_{i=1}^n 2(a_2x_i^2 + a_1x_i + a_0 - y_i) &= 0 \end{aligned} \quad (26.24)$$

Equation (26.24) represents a set of three equations containing unknowns  $a_0$ ,  $a_1$ , and  $a_2$ . Recasting these in matrix form gives

$$\begin{bmatrix} n & \sum_{i=1}^n x_i & \sum_{i=1}^n x_i^2 \\ \sum_{i=1}^n x_i & \sum_{i=1}^n x_i^2 & \sum_{i=1}^n x_i^3 \\ \sum_{i=1}^n x_i^2 & \sum_{i=1}^n x_i^3 & \sum_{i=1}^n x_i^4 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^n y_i \\ \sum_{i=1}^n x_i y_i \\ \sum_{i=1}^n x_i^2 y_i \end{bmatrix} \quad (26.25)$$

Equation (26.25) may then be solved for the regression coefficients  $a_0$ ,  $a_1$ , and  $a_2$ .<sup>(12)</sup>

The above development can easily be extended to other types of polynomials. Other functions are listed below.

$$\begin{aligned} 0\text{th degree polynomial: } y &= a_0 \\ 1\text{st degree polynomial: } y &= a_0 + a_1x_1 \\ 2\text{nd degree polynomial: } y &= a_0 + a_1x_1 + a_2x_2^2 \\ m\text{th degree polynomial: } y &= a_0 + a_0x_1 + \cdots + a_0x_m^m \end{aligned} \quad (26.26)$$

The above can also be applied to functions  $f_i(x)$  that are complex. For example, if

$$y = a_1f_1(x) + a_2f_2(x) + a_3f_3(x) \quad (26.27)$$

then Equation (26.27) takes the form:

$$\begin{bmatrix} \sum f_1^2 & \sum f_1f_2 & \sum f_1f_3 \\ \sum f_1f_2 & \sum f_2^2 & \sum f_2f_3 \\ \sum f_1f_3 & \sum f_2f_3 & \sum f_3^2 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} \sum y_i f_1 \\ \sum y_i f_2 \\ \sum y_i f_3 \end{bmatrix} \quad (26.28)$$

The reader is referred to Illustrative Example 28.4 for additional details.

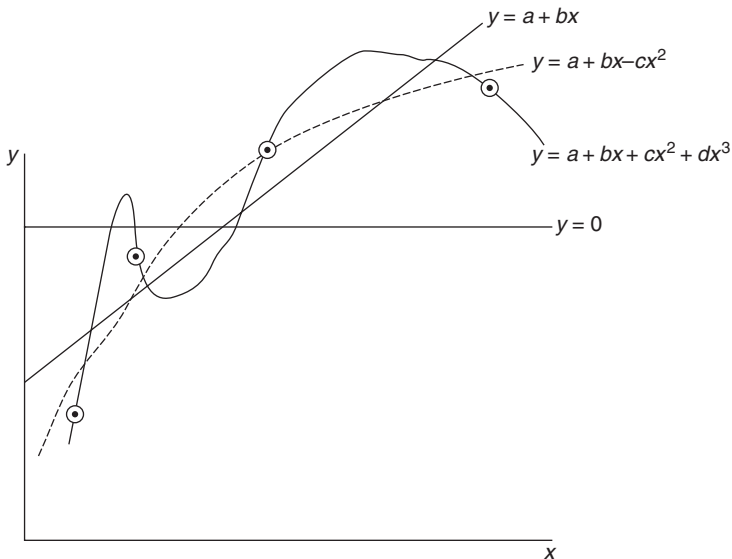


## Correlation Coefficient

When data is plotted to determine any possible relationship, it is common to try to fit the data to some sort of curve (typically a line). The correlation coefficient is a measure of the amount of deviation between the variables. A correlation coefficient of 1.0 indicates a perfect association between the variables; a correlation coefficient of 0.0 indicates a completely random relation. Nothing is said about the dependence or independence of the variables, and nothing is said about the nature of the relation between the variables.

Although the correlation coefficient provides an answer as to how well the model fits the data, it does not provide an answer as to whether it is the best and/or correct model. In fact, it can often provide misleading information. For example, if one were interesting in fitting a model to the four data points presented in Figure 26.8, one could apply a zero, first, second or third order model to the data. These four models are superimposed on the figure. The zero order polynomial would provide the worst correlation coefficient while the third order polynomial (which exactly passes through each data point) would correlate perfectly with a corresponding correlation coefficient of 1.0. Obviously, the latter is almost certainly *not* the “correct” or “best” model.<sup>(12)</sup>

To obtain information on the “best” model, one must resort to a statistical technique referred to as ANOVA, an acronym referring to Analysis Of Variance. This topic is beyond the scope of this text; however, information is available in the literature.<sup>(12,13)</sup>



**Figure 26.8** Regression models.

**ILLUSTRATIVE EXAMPLE 26.8**<sup>(14)</sup>

Species  $A$  is undergoing a reaction in a tubular flow unit. The following data (see Table 26.1) have been obtained for the rate,  $-r_A$ , versus concentration,  $C_A$ . Using this data, estimate the coefficient  $k_A$  and  $\alpha$  in the equation below.

$$-r_A = k_A C_A^\alpha$$

**SOLUTION:** Linearize the describing equation

$$\ln(-r_A) = \ln(k_A) + \alpha \ln(C_A)$$

Change the variables to  $Y$  and  $X$ .

$$Y = A + BX$$

where

$$Y = \ln(-r_A)$$

$$A = \ln(k_A)$$

$$B = \alpha$$

Substitute the above data.

$$\ln(3) = A + B \ln(2)$$

$$\ln(12) = A + B \ln(4)$$

$$\ln(27) = A + B \ln(6)$$

$$\ln(48) = A + B \ln(8)$$

Generate the linear coefficients  $A$  and  $B$  using any convenient method:

$$A = -0.2878$$

$$B = 2.0$$

Therefore,

$$k_A = 0.75$$

$$\alpha = 2.0$$

and the equation for the rate of reaction is

$$-r_A = 0.75 C_A^2$$

**Table 26.1** Rate Data; illustrative Example 26.8

$-r_A$ , lbmol/ft <sup>3</sup> · s	$C_A$ , lbmol/ft <sup>3</sup>
48	8
27	6
12	4
3	2

Obviously, the regression of data has been greatly simplified through the use of software packages. ■

### ILLUSTRATIVE EXAMPLE 26.9

The viscosity of air as a function of temperature is provided below in Table 26.2. Assuming a linear relationship, obtain the viscosity as a function of temperature.

**SOLUTION:** For a linear model,

$$\mu = A + BT$$

Regressing the data using the method of least squares gives

$$A = 1.7456$$

$$B = 0.0083$$

Therefore,

$$\mu = 1.7456 + 0.0083T$$

with  $\mu$  in  $\text{kg/m} \cdot \text{s} \times 10^5$  and  $T$  in  $^{\circ}\text{C}$ .

**Table 26.2** Viscosity–Temperature Data; Illustrative Example 26.9

Temperature, $T$ , $^{\circ}\text{C}$	Viscosity, $\mu$ , $\text{kg/m} \cdot \text{s} \times 10^5$
−40	1.51
−20	1.61
0	1.71
10	1.76
12	1.81
30	1.86
40	1.90
50	1.95
60	2.00
80	2.09
100	2.17
150	2.38
200	2.57
250	2.75
300	2.93
400	3.25
500	3.55

## OPTIMIZATION

Optimization has come to mean different things to different people. However, one might offer the following generic definition: “*Optimization* is concerned with determining the ‘best’ solution to a given problem”. This process is required in the solution of many problems that involves the maximization or minimization of a given function.

A significant number of optimization problems face the practicing engineer. The optimal design of industrial processes as well as heat exchangers has long been of concern to the practicing engineer, and indeed, for some, might be taken as a definition of the function and goal of applied engineering. The practical attainment of an optimum design is generally a result of factors that include mathematical analysis, empirical information, and both the subjective and objective experience of the engineer.

In a general sense, optimization problems can be divided into four categories:

1. The number of independent variables involved.
2. Whether the optimization is “constrained.”
3. Time-independent systems.
4. Time-dependent systems.

In addition, if no unknown factors are present, the system is defined as *deterministic* while a system containing experimental errors and/or other random factors is defined as *stochastic*.

### Perturbation Studies in Optimization

Once a particular heat exchange or process scheme has been selected, 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 to a heat exchanger analysis. These sophisticated optimization techniques, some of which are also routinely used in the design of conventional chemical and petrochemical plants, invariably involve computer calculations. Use of these techniques in heat exchanger analysis is not always warranted, however.

One simple optimization procedure that is recommended is the *perturbation study*. This involves a systematic change (or *perturbation*) of variables, one by one, in an attempt to locate the optimum design from a cost and operation viewpoint. To be practical, this often means that the engineer must limit the number of variables by assigning constant values to those process variables that are known beforehand to play an insignificant role. Reasonable guesses and simple or short-cut mathematical methods can further simplify the procedure. Much information can be gathered from this type of study since it usually identifies those variables that significantly impact on the overall performance of the heat exchanger or process and also helps identify the major contributors in the procedure.

More detailed and sophisticated optimization procedures are available, most of which are located in the literature.<sup>(15,16)</sup> Three illustrative examples follow, two

additional illustrative examples that outline the methodology employed in optimization calculations can be found later in Chapter 27. As is often the case, both examples involve an economic analysis.

### ILLUSTRATIVE EXAMPLE 26.10

Qualitatively describe the objective of rigorous optimization techniques.<sup>(15)</sup>

**SOLUTION:** Formal optimization techniques have as their goal the development of procedures for the attainment of an optimum in a system which can be characterized mathematically. The mathematical characterization may be:

1. partial or complete
2. approximate or exact, and/or
3. empirical or theoretical.

The resulting optimum may be a final implementable design or a guide to practical design and a criterion by which practical designs are to be judged. In either case, the optimization techniques should serve as an important part of the total effort in the design of the units, structure, and control of a industrial system, including heat exchangers. ■

### ILLUSTRATIVE EXAMPLE 26.11

A refinery has two catcrackers that can produce various grades of hydrocarbon products. Because of consumer fuel demand, the production of gasoline, home heating oil and diesel must be limited. This information is provided in Table 26.3.

The profit on processing U.S. crude oil is \$2.00/gal and on Venezuelan crude is \$1.60/gal. Find the approximate daily processing rate of the two crudes in order to maximize profits.

**SOLUTION:** Set

$q_1$  = gallons of U.S. crude

$q_2$  = gallons of Venezuelan crude

The objective function for the daily profit,  $P$ , that is to be maximized is:

$$P = 2.0q_1 + 1.6q_2$$

**Table 26.3** Cat Cracker Information

Product grades	U.S. crude (% distribution)	Venezuelan crude (% distribution)	Max. production rate (gal/day)
Gasoline	8	11	1500
Home heating oil	29	54	5500
Diesel oil	63	35	11,000

The constraints are:

$$\begin{aligned}0.08q_1 + 0.11q_2 &\leq 1500 \\0.29q_1 + 0.54q_2 &\leq 5500 \\0.63q_1 + 0.35q_2 &\leq 11,000 \\q_1 \geq 0, q_2 &\geq 0\end{aligned}$$

The solution to the above from Excel is: 16,820 gal of U.S. crude per day should be processed and 1152 gal per day should be derived from Venezuelan crude. This results in a total daily profit of \$35,484.<sup>(17)</sup> ■

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