CHAPTER 1

Review of Mathematical Principles and Applications in Food Processing

1.1 GRAPHING AND FITTING EQUATIONS TO EXPERIMENTAL DATA

1.1.1 Variables and Functions

A variable is a quantity that can assume any value. In algebraic expressions, variables are represented by letters from the end of the alphabet. In physics and engineering, any letter of the alphabet and Greek letters are used as symbols for physical quantities. Any symbol may represent a variable if the value of the physical quantity it represents is not fixed in the statement of the problem. In an algebraic expression, the letters from the beginning of the alphabet often represent constants; that is, their values are fixed. Thus, in the expression $ax = 2by$, x and y represent variables and a and b are constants.

A function represents the mathematical relationship between variables. Thus, the temperature in a solid that is being heated in an oven may be expressed as a function of time and position using the mathematical expression $T = F(x, t)$. In an algebraic expression, $y = 2x + 4$, $y = F(x)$, and $F(x) = 2x + 4$.

Variables may be dependent or independent. Unless defined, the dependent variable in a mathematical expression is one that stands alone on one side of an equation. In the expression $y = F(x)$, y is the dependent and x is the independent variable. When the expression is rearranged in the form $x = F(y)$, x is the dependent and y is the independent variable. In physical or chemical systems, the interdependence of the variables is determined by the design of the experiment. The independent variables are those fixed in the design of the experiment, and the dependent variables are those that are measured. For example, when determining the loss of ascorbic acid in stored canned foods, ascorbic acid concentration is the dependent variable and time is the independent variable. On the other hand, if an experiment involves taking a sample of a food and measuring both moisture content and water activity, either of these two variables may be designated as the dependent or independent variable. In statistical design, the terms “response variable” and “treatment variable” are used for the dependent and independent variables, respectively.

1.1.2 Graphs

Each data point obtained in an experiment is a set of numbers representing the values of the independent and dependent variables. A data point for a response variable that depends on only one independent variable (univariate) will be a number pair, whereas with response variables that depend on several independent variables (multivariate), a data point will consist of a value for the response variable and one value each for the treatment variables. Experimental data are often presented as a table of numerical values of the variables or as a graph. The graph traces the path of the dependent variable as the values of the independent variables are changed. For univariate responses, the graph will be two-dimensional, and multivariate responses will be represented by multidimensional graphs.

When all variables in the function have the exponent of one, the function is called first order and will be represented by a straight line. When any of the variables has an exponent other than one, the graph will be a curve in rectangular coordinates.

The numerical values represented by a data point are called the "coordinate" of that point. When plotting experimental data, the independent variable is plotted on the horizontal axis or "abscissa" and the dependent variable is plotted on the vertical axis or "ordinate." The rectangular or Cartesian coordinate system is the most common system for graphing data. Both abscissa and ordinate are in the arithmetic scale and the distance from the origin measured along or parallel to the abscissa or ordinate to the point under consideration is directly proportional to the value of the coordinate of that point. Scaling of the abscissa and ordinate is done such that the data points, when plotted, will be symmetrical and centered within the graph. The Cartesian coordinate system is divided into four quadrants with the origin in the center. The upper right quadrant represents points with positive coordinates, the left right quadrant represents negative values of the variable on the abscissa and positive values for the variable on the ordinate, the lower left quadrant represents negative values for both variables, and the lower right quadrant represents positive values for the variable on the abscissa and negative values for the variable on the ordinate.

1.1.3 Equations

An equation is a statement of equality. Equations are useful for presenting experimental data because they can be mathematically manipulated. Furthermore, if the function is continuous, interpolation between experimentally derived values for a variable may be possible. Experimental data may be fitted to an equation using any of the following techniques:

1. Linear and polynomial regression: Statistical methods are employed to determine the coefficients of a linear or polynomial expression involving the independent and dependent variables. Statistical procedures are based on minimizing the sum of squares for the difference between the experimental values and values predicted by the equation.
2. Linearization, data transformation, and linear regression: The equation to which the data is being fitted is linearized. The data is then transformed in accordance with the linearized equation, and a linear regression will determine the appropriate coefficients for the linearized equation.
3. Graphing: The raw or transformed data is plotted to form a straight line, and from the slopes and intercept the coefficients of the variables in the equation are determined.

1.1.4 Linear Equations

Plotting of linear equations can be facilitated by writing the equation in the following forms:

1. The slope-intercept form: $y = ax + b$, where $a =$ the slope, and $b =$ the y-intercept, or the point on the ordinate at $x = 0$. The slope is determined by taking two points on the line with coordinates (x_1, y_1) and (x_2, y_2), and solving for $a = (y_2 - y_1)/(x_2 - x_1)$.
2. The point-slope form: $(y - b) = a\,(x - c)$, where $a =$ slope, and b, c represent coordinates of a point (c, b) through which the line must pass. When linear regression is used on experimental data, the slope and the intercept of the line are calculated. The line must pass through the point that represents the mean of x and the mean of y. A line can then be drawn easily using either the point-slope or the slope-intercept forms of the equation for the line.

The equations for slope and intercept of a line obtained by regression analysis of N pairs of experimental data are

$$a = \frac{\sum xy - \left(\sum x \sum y\right)/N}{\sum x^2 - \left[\left(\sum x\right)^2/N\right]};\quad b = \frac{\sum y \sum x^2 - \sum x \sum xy}{N\left(\sum x^2 - \left[\left(\sum x\right)^2/N\right]\right)}$$

The process of regression involves minimizing the square of the difference between value of y calculated by the regression equation and y_i, the experimental value of y. In linear regression, $\Sigma(ax + b - y)^2$ is called the explained variation, and $\Sigma(y_i - y)^2$ is called the random error or unexplained variation.

The ratio of the explained and unexplained variation is called the correlation coefficient. If all the points fall exactly on the regression line, the variation of y from the mean will be due to the regression equation, therefore explained variation equals the unexplained variation, and the correlation coefficient is 1.00. If there is too much data scatter, the random or unexplained variation will be very large, and the correlation coefficient will be less than 1.00. Thus, regression analysis not only determines the equation of a line that fits the data points, but it can also be used to test if a predictable relationship exists between the independent and dependent variables. The formula for the linear correlation coefficient is

$$r = \frac{N\sum xy - \sum x \sum y}{\left[\left[N\sum x^2 - \left(\sum x\right)^2\right]\left[N\sum y^2 - \left(\sum y\right)^2\right]\right]^{0.5}}$$

r will have the same sign as the regression coefficient a. Values for r that is much different from 1.0 must be tested for significance of the regression. The student is referred to statistics textbooks for procedures to follow in testing significance of regression from the correlation coefficient.

Example 1.1. The protein efficiency ratio (PER) of a protein is defined as the weight gain of an animal fed a diet containing the test protein per unit weight of protein consumed. Data is collected by providing feed and water to the animal so the animal can feed at will, determining the amount of feed consumed, and weighing each animal at designated time intervals. The PER may be calculated from the slope of the regression line for weight of the animal (y) against cumulative weight of protein consumed (x). The data expressed as (x, y) where x is the amount of feed consumed and y is the weight are as follows: (0, 11.5), (0, 12.2), (0, 14.0), (0, 13.3), (0, 12.5), (2.0, 16.8), (2.2, 16.7), (1.8, 15.2), (2.5, 18.4), (1.8, 16.8), (3.4, 22.8), (4.2, 22.5), (3.7, 20.7), (4.6, 25.3), (4.0, 23.5), (6.5, 28.0), (6.3, 29.5), (6.8, 31.0), (5.8, 28.5), (6.6, 29.0).

Perform a regression analysis and determine the PER.

Solution:

The sum and sums of squares of the x and y are $\Sigma x = 62.2$; $\Sigma x^2 = 307.00$; $\Sigma y = 408.2$; $\Sigma y^2 = 9138.62$; $\Sigma xy = 1568.28$; $N = 20$. The mean of $x = \Sigma x/N = 62.2/20 = 3.11$.

$$a = \frac{408.2 - (62.2)(408.20/20)}{307.00 - (62.20)^2/20} = 2.631$$

$$b = \left(\frac{1}{20}\right)\left[\frac{(408.20)(307.00) - (62.20)(1568.28)}{307.00 - (62.20)^2/20}\right] = 12.23$$

The mean of $y = \Sigma y/N = 408.2/20 = 20.41$. Thus the best-fit line will go through the point (3.11, 20.41).

The correlation coefficient "r" is calculated as follows:

$$r = \frac{20(1568.28) - 62.2(408.20)}{[[20(307.00) - (62.20)^2][20(9138.62) - (408.20^2]]^{0.5}}$$

$$r = 0.9868$$

The correlation coefficient is very close to 1.0, indicating very good fit of the data to the regression equation. The regression and graphing can also be performed using a spreadsheet as discussed later in this chapter. The PER is the slope of the line, 2.631.

1.1.5 Nonlinear Equations

Nonlinear monovariate equations are those where the exponent of any variable in the equation is a number other than one. The polynomial: $y = a + bx + cx^2 + dx^3$ is often used to represent experimental data. The term with the exponent 1 is the linear term. that with the exponent 2 is the quadratic term, and that with the exponent 3 is the cubic term. Thus b, c, and d are often referred to as the linear, quadratic, and cubic coefficients, respectively. Linear regression analysis is used to determine the coefficients of a polynomial that fits the experimental data. Although the polynomial is nonlinear, linear regression analysis is used because the first partial derivative of the function with respect to any of the coefficients is a constant. The objective of polynomial regression is to determine the coefficients of the polynomial such that the sum of the squares of the difference between experimental and predicted value of the response variable is a minimum. Polynomial regression is more difficult to perform manually than linear regression because of the number of coefficients that must be evaluated. Stepwise regression analysis may be performed, that is, additional terms are added to the polynomial, and the contribution of each additional term in reducing the error sum of squares is evaluated. To illustrate the complexity of polynomial compared with linear regression, the equations that must be solved to determine the coefficients are as follows:

For linear regression, $y = ax + b$:

$$\Sigma y = aN + b\Sigma x$$

$$\Sigma xy = aN\ \Sigma x + b\Sigma x^2$$

For a second-order polynomial, $y = a + bx + cx^2$:

$$\Sigma\, y = aN + b\Sigma x + c\Sigma x^2$$
$$\Sigma\, xy = aN\Sigma x + b\Sigma x^2 + c\Sigma x^3$$
$$\Sigma\, x^2 y = aN\Sigma x^2 + b\Sigma x^3 + c\Sigma x^4$$

Thus, evaluation of coefficients for the linear regression is relatively easy, involving the solution of two simultaneous equations. On the other hand, polynomial regression involves solving $n + 1$ simultaneous equations to evaluate coefficients of an *n*th order polynomial. Determinants can be used to determine the constants for an *n*th order polynomial. Techniques for solving determinants manually and using a spreadsheet program are discussed later in this chapter. For the second-order polynomial (quadratic) equation, the constants a, b, and c are solved by substituting the values of N, Σx, Σx^2, Σx^3, Σx^4, Σxy, and $\Sigma x^2 y$, into the three equations above and solving them simultaneously.

1.2 LINEARIZATION OF NONLINEAR EQUATIONS

Nonlinear equations may be linearized by series expansion, but the technique is only an approximation and the result is good only for a limited range of values for the variables. Another technique for linearization involves mathematical manipulation of the function and transformation and/or grouping such that the transformed function assumes the form:

$$F(x, y) = aG(x, y) + b$$

where a and b are constants whose values do not depend on x and y.

Example 1.2. $xy = 5$.

Linearized form: $y = 5\left(\frac{1}{x}\right)$

A plot of y against (1/x) will be linear.

Example 1.3.

$y = (y^2/x) + 4.$

$y^2 = xy - 4x \qquad y^2 = x(y - 4)$ A plot of x against $y^2/(y - 4)$ will be linear

Example 1.4. The hyperbolic function $y = 1/(b + x)$.

$$\frac{1}{y} = b + x$$

A plot of 1/y against x will be linear.

Example 1.5. The exponential function $y = ab^x$.

$$\log y = \log a + x \log b$$

A plot of log y against x will be linear.

Example 1.6. The geometric function $y = ax^b$.

$\log y = \log a + b \log x$

A plot of log y against log x will be linear.

1.3 NONLINEAR CURVE FITTING

Linearizing an equation and fitting the linearized equation to the data has the advantage of simplicity but will require several replicates of entire data sets in order to be able to obtain reliable estimates of confidence limits for the equation parameters. Linearization also introduces complex errors particularly when two measured variables both appear in a linearized term. Nonlinear curve-fitting techniques permits determination of parameter estimates and their confidence interval from a single data set consisting of numerous data points. There are several nonlinear curve-fitting routines available. One commonly used software is Systat. To use Systat for data analysis, the data must be entered or imported into a Systat worksheet and saved as a Systat file.

To use Systat, first access the program and open the Systat main menu. Select *Window* and on the pop-up menu, select *Worksheet.* Data may then be entered in the worksheet. The first row should be the variable's name, and the values are entered in the column corresponding to the variables. Data may then be saved by selecting *File* and *Save*. Exit the worksheet by choosing the "X" (exit) button and return to the Systat main menu. To use data files saved in the Systat directory, chose *Open* in the *Worksheet* menu. Enter the *Filename* with the *.sys* extension and chose *Edit*. The system will return to the Systat Main menu and the following message is displayed: "Welcome to Systat. Systat variables available to you are." If a printout of the confidence interval of the parameter estimates is desired, select *Data* in the main menu and select *Format* in the pop-up menu. Then select *Extended (Long)* and *OK* to get back to the main menu. The Systat toolbar then becomes active. Select *Stats* in the Systat Main menu and select *Nonlin* in the pop-up menu. Follow the prompts. First select *Loss Function* and enter Loss function that is to be minimized. Usually this will be the sum of squares of the value of the dependent variable and the estimate. Although the sum of squares is the default, sometimes the program does not do the required iterations if nothing is entered for the loss function. Then select *OK* and when the display returns to the Systat Main menu, select *Stats* again, select *Nonlin* in the pop-up menu, and select *Model*. Enter the model desired for fitting into the data. Enter initial values of the coefficients separated by commas. Enter number of iterations. Select *OK* and Systat will return values of the parameter estimates and the loss function.

Example 1.7. Data on degradation of neoaxanthin, a carotenoid pigment in olives [*J. Agric. Food Chem.* (1994) 42:1551–1554] is as follows [Days, Conc. (in mg/kg)]: (0, 1.41), (4, 1.29), (8, 1.18), (14, .98), (19, 0.80), (20, 0.76), (26, 0.62), (33; 0.51), (54, 0.13). The change of concentration with time is first order, therefore the logarithm of concentration when plotted against time is linear. Fit the logarithmic equation $\ln(C) = kt + b$ by linear regression to obtain parameter estimates of k and b. Also fit the equation $C = [e]^{kt+b}$ and obtain parameter estimates of k and b and their confidence limits using nonlinear curve fitting.

Solution:

Enter the data into the worksheet, save and exit. The Systat main menu will indicate that the following variables are available: "Days and Neo." Select *Data*, then *Format*, then *Extended (long)*, and *OK*.

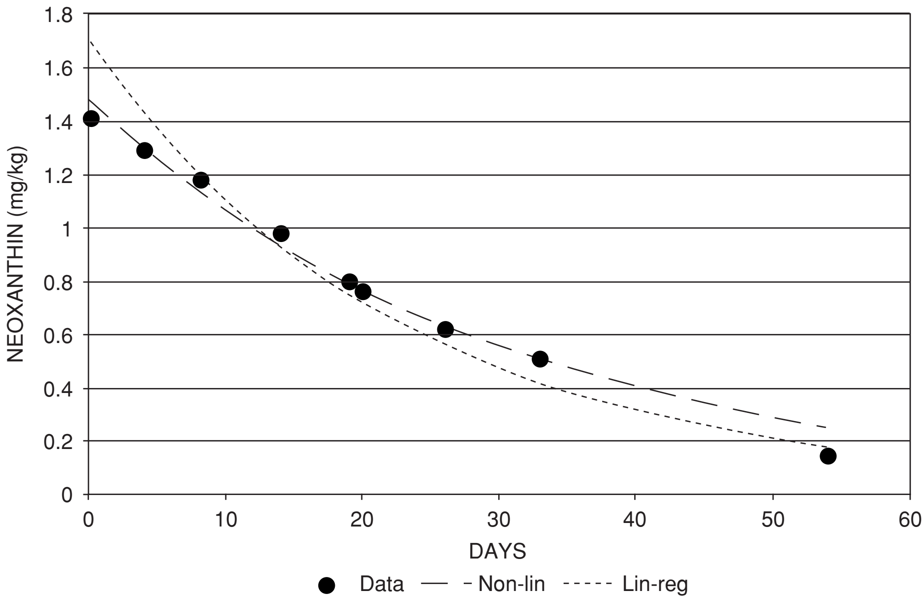

Figure 1.1 Graph showing fit to experimental data of a first-order equation with model parameters determined using linearization and linear regression (Lin-reg) and nonlinear curve fitting (Non-lin).

Back into the Systat main menu, select *Stats* then *Nonlin* and *Loss Function*. Enter "(Neo–estimate) ^2" in the loss function expression box and select *OK*. Back in the Systat main menu, select *Stats*, then *Nonlin*, then *Model*. Enter "neo = exp(k*days + b)" in the *Model* expression box, −1, 1 in the *Start* box, and 20 in the *Iterations* box. Select *OK*. Parameter estimates k = −0.033 ∀ .005 and b = 0.387 ∀ .066 and a loss function of .023 are displayed. To ensure that this is not a local minimum for the loss function, select *Stats*, then *Nonlin*, then *Resum*e. Enter −.1 and 0.5 in the *Start* box and 20 in the *Iterations* box. Select *OK*. Displayed values of k and b are the same as above.

To fit a linearized form of the first-order equation, use ln(neo) = k*days + b. Transform the values for concentration of neoxanthin into their natural logarithms and perform a linear regression. This may be done using the *Regrn* function of Systat or the Statistics routine in Excel. Using Systat, enter the values of log(neo) at indicated days in the worksheet, and save. The Systat main menu then appears. Select *Regrn*. Select logneo as the dependent and days as the independent variable. Select *OK*. Systat displays −0.043 as the slope and 0.521 as the constant. The correlation coefficient is 0.958 showing reasonably good fit of the linearized equation to the data.

Figure 1.1 shows a plot of the experimental data and the fitted equations. The nonlinear curve-fitted parameters show closer values to the experimental data than the linearized transformed variable fitted parameters. Linearization forced the function to be strongly influenced by the last data point resulting in underestimation of the middle and overestimation of the first few data points. Nonlinear curve fitting is recommended over linearization, when possible.

The solver feature of Microsoft Excel may also be used to do the curve fitting. An example of how Excel may be used for curve fitting to determine kinetic parameters is shown in the section "Determining Kinetic Parameters" in Chapter 8.

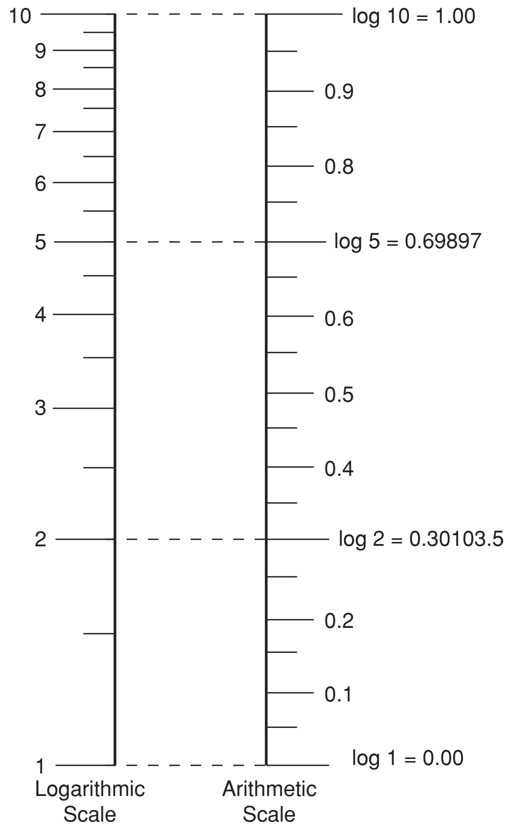

Figure 1.2 Scaling of logarithmic scale used on the logarithmic axis of semi-logarithmic or full logarithmic graphing paper.

1.4 LOGARITHMIC AND SEMI-LOGARITHMIC GRAPHS

Graphing paper is available in which the ordinate and abscissa are in the logarithmic scale. A full logarithmic or log-log graphing paper has both abscissa and ordinate in the logarithmic scale. A semi-logarithmic graphing paper has the ordinate in the logarithmic scale and the abscissa in the arithmetic scale. Full logarithmic graphs are used for geometric functions as in Example 1.6 above, and semi-logarithmic graphs are used for exponential functions as in Example 1.5. The distances used in marking coordinates of points in the logarithmic scale are shown in Fig. 1.2. Each cycle of the logarithmic scale is marked by numbers from 1 to 10. Distances are scaled on the basis of the logarithm of numbers to the base 10. Thus, there is a repeating cycle with multiples of 10. One cycle semi-logarithmic and full logarithmic graphing paper is shown in Fig. 1.3.

When plotting points on the logarithmic scale, label the extreme left and lower coordinates of the graph with the multiple of 10 immediately below the magnitude of the least coordinate to be graphed. Thus, if the least magnitude of the coordinate of the point to be plotted is 0.025, then the extreme left or lower coordinate of the graph should be labeled 0.01. The number of cycles on the logarithmic scale of the graph to be used must be selected such that the points plotted will occupy most of the graph

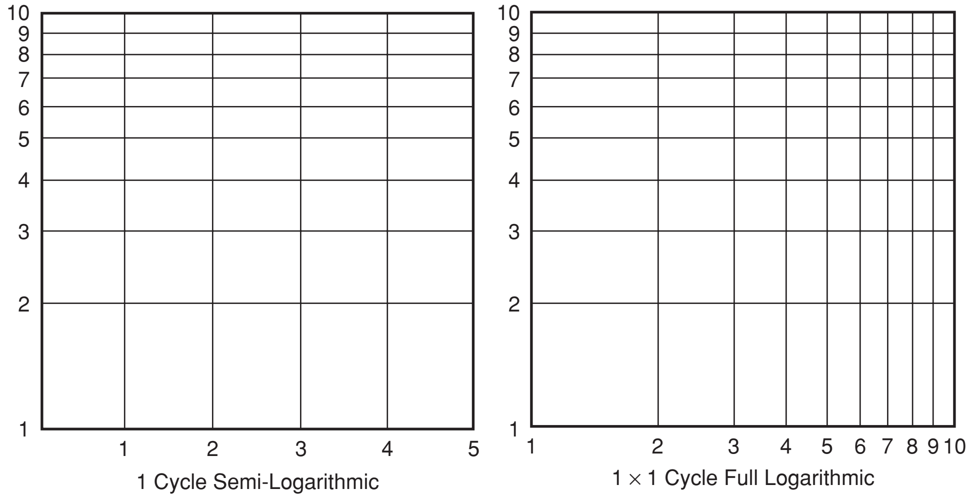

Figure 1.3 One cycle semi-logarithmic and full logarithmic graphing paper.

after plotting. Thus, if the range of numbers to be plotted is from 0.025 to 3.02, three logarithmic cycles will be needed (0.01 to 0.1; 0.1 to 1; 1 to 10). If the range of numbers is from 1.2 to 9.5, only one cycle will be needed (1 to 10).

Numerical values of data points are directly plotted on the logarithmic axis. The scaling of the graph accounts for the logarithmic relationship. Thus, points, when read from the graph, will be in the original rather than the logarithmically transformed data.

$$\text{Slope} = \frac{\log\ y_2 - \log\ y_1}{\log x_2 - \log x_1}$$

Slopes on log-log graphs are determined using the following formula:
Coordinates of points (x_1, y_1) and (x_2, y_2), which are exactly on the line drawn to best fit the data points, are located. Enough separation should be provided between the points to minimize errors. At least one log cycle separation should be allowed on either the ordinate or abscissa between the two points selected.

Slopes on semi-logarithmic graphs are calculated according to the following formula:

$$\text{Slope} = \frac{\log y_2 - \log y_1}{x_2 - x_1}$$

A separation of at least one log cycle, if possible, should be allowed between the points (x_1, y_1) and (x_2, y_2). Figure 1.4 shows the logarithmic scale relative to the arithmetic scale that would be used if the data is transformed to logarithms prior to plotting. The determination of the slope and intercept is also shown.
The following examples illustrate the use of semi-log and log-log graphs:

Example 1.8. An index of the rate of growth of microorganisms is the generation time (g). In the logarithmic phase of microbial growth, number of organisms (N) change with time of growth (t) according to:

$$N = N_o[2]^{t/g}$$

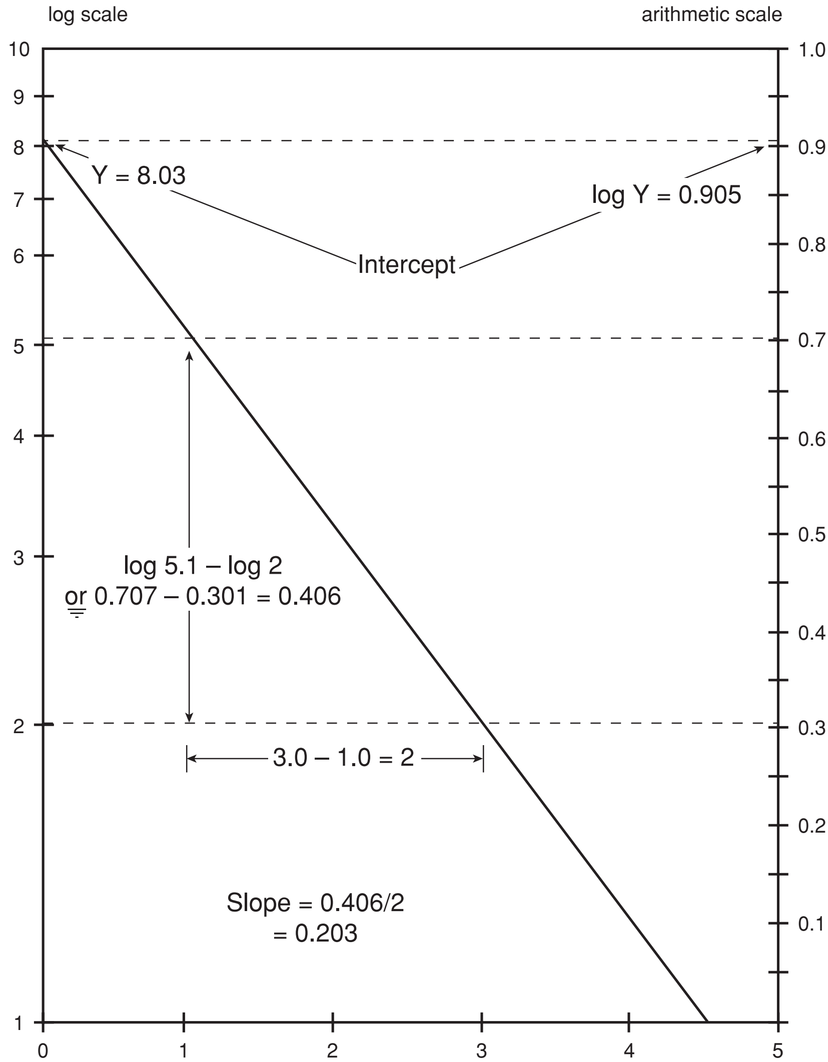

Figure 1.4 Graph showing the logarithmic relative to the arithmetic scale, and how the slope and intercept are determined on a semi-logarithmic graph.

Find the generation time of a bacterial culture that shows the following numbers with time of growth:

Numbers (N)	*Time of growth, (t), in minutes*
980	0
1700	10
4000	30
6200	40

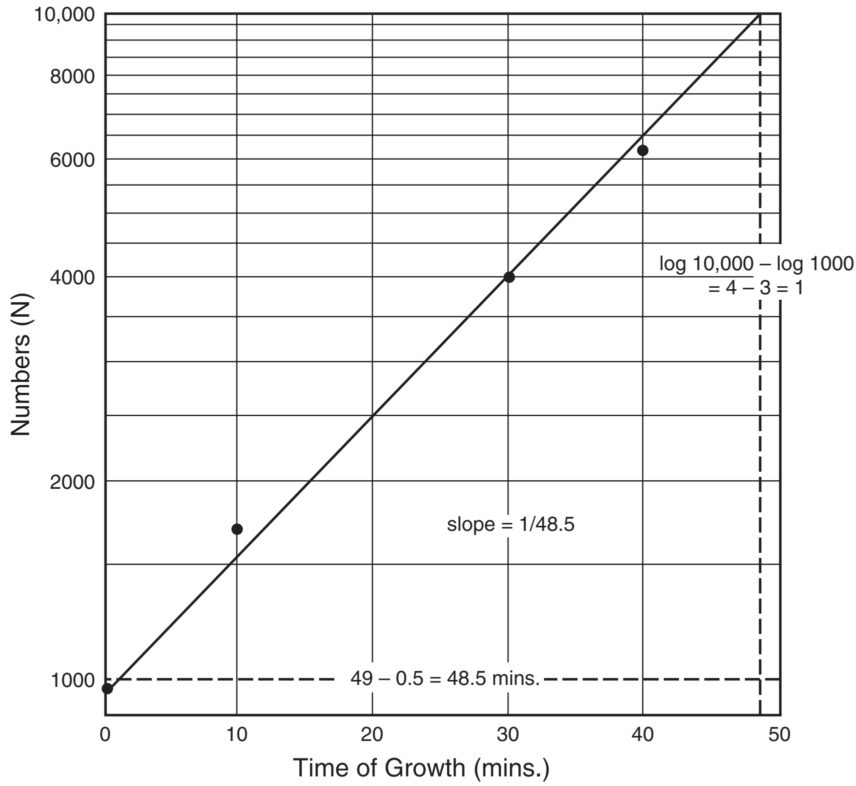

Figure 1.5 Semi-logarithmic plot of microbial growth.

Solution:

Taking the logarithm of the equation for cell numbers as a function of time:

$$\text{Slope} = \frac{\log 2}{g}$$

$$\log N = \log No + (t/g)\log 2$$

Plotting log N against t will give a straight line. A semi-logarithmic graphing paper is required for plotting. The slope of the line will be from Fig. 5, the two points selected to obtain the slope are (0,1000) and (48.5,10000). The two points are separated by one log cycle on the ordinate. The slope is $1/48.5 = 0.0206\ \text{min}^{-1}$. The generation time $g = \log 2/\text{slope} = 14.6$ minutes.

Regression eliminates the guesswork in locating the position of the best-fit line among the data points. Let $\log(N) = y$ and $t = x$. The sums are $\Sigma x = 80$, $\Sigma y = 13.616$, $\Sigma x^2 = 2600$, $\Sigma y^2 = 46.740$, $\Sigma xy = 292.06$.

$$a = \frac{292.06 - 80(13.616)/4}{2600 - (80)^2/4} = 0.01974$$

$$b = \frac{13.616(2600) - 80(292.06)}{4[2600 - (80)^2/4]} = 3.0092$$

The graph is shown in Fig. 1.5. A best-fit line is drawn by positioning the straight edge such that points below the line balance those above the line. Although the equation for N suggests that any two data points may be used to determine g, it is advisable to plot the data to make sure that the two points selected lie exactly on the best-fitting line.

The correlation coefficient is:

$$r = \frac{4(292.06 - 80(13.616)}{\left([4(2600) - (80)^2][4(46.740) - (13.616)^2]\right)^{0.5}} = 0.9981$$

The correlation coefficient is very close to 1.0, indicating good fit of the data to the regression equation. The slope is 0.01974. g = log (2)/0.01974 = 15.2 minutes.

The parameter estimate for g by nonlinear curve fitting using Systat and the model [$N =$ 980*10^(time/g)] returns a parameter estimate for g of 14.834 ∀ 0.997.

Example 1.9. The term "half-life" is an index used to express stability of a compound and is defined as the time required for the concentration to drop to half the original value. In equation form:

$$C = C_o[2]^{-t/t_{0.5}}$$

where Co is concentration at t = 0, C is concentration at any time t, and $t_{0.5}$ is the half-life.

Ascorbic acid in canned orange juice has a half-life of 30 weeks. If the concentration just after canning is 60 mg/100 mL, calculate the concentration after 10 weeks. When labeling the product, the concentration declared on the label must be at least 90% of the actual concentration. What concentration must be declared on the label to meet this requirement at 10 weeks of storage?

Graphical Solution:

A logarithmic transformation of the equation for concentration as a function of time results in:

$$\log C = \log C_o - \left[\frac{\log 2}{t_{0.5}}\right] t$$

A plot of C against t on semi-logarithmic graphing paper will be linear with a slope of $-(\log 2)/t_{0.5}$.

Figure 1.6 is a graph constructed by plotting 60 mg/100 mL at t = 0 and half that concentration (30 mg/100 mL) at t = 30 weeks and drawing a line connecting the two points. At t = 10 weeks, a point on the line shows a concentration of 47.5 mg/100 mL. Thus, a concentration of 0.9(47.5) or 42.9 mg/100 mL would be the maximum that can be declared on the label.

Analytical Solution:

Given: $C_o = 60$; $t_{0.5} = 30$; at t = 10, C_{10} = concentration and the declared concentration on the label, $C_d = 0.9\ C_{10}$. Solving for C_d:

$$C_d = 0.9(60)[2]^{-10/30}$$
$$= 0.9(60)(0.7938) = 42.86 \text{ mg/mL}$$

Example 1.10. The pressure-volume relationship that exists during adiabatic compression of a real gas is given by $PV^n = C$, where P is absolute pressure, V is volume, n is the adiabatic expansion factor,

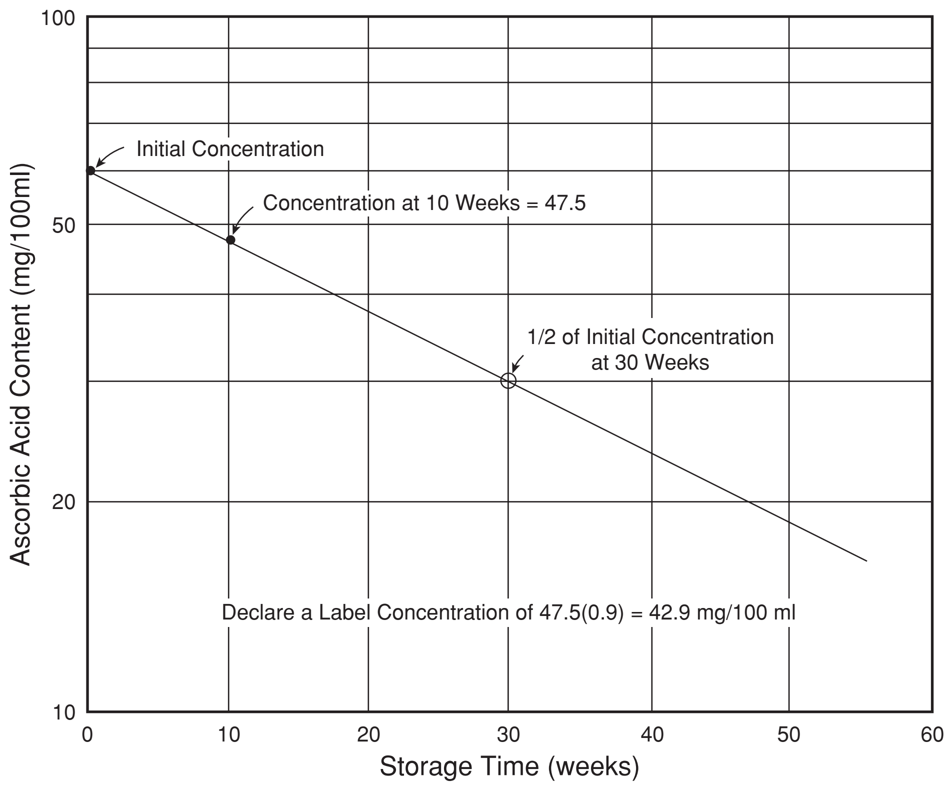

Figure 1.6 Graphical representation of the half-life illustrated by ascorbic acid degradation with time of storage.

and C is a constant. Calculate the value of the adiabatic expansion factor, n, for a gas that exhibits the following pressure-volume relationship:

Volume (ft^3)	Absolute Pressure ($lb_f/in.^2$)
53.3	61.2
61.8	49.5
72.4	37.6
88.7	28.4
118.6	19.2
194.0	10.1

Solution:

The equation may be linearized and the value of n determined from the linear plot of the data. Taking the logarithm:

$$\log P = -n \log V + \log C$$

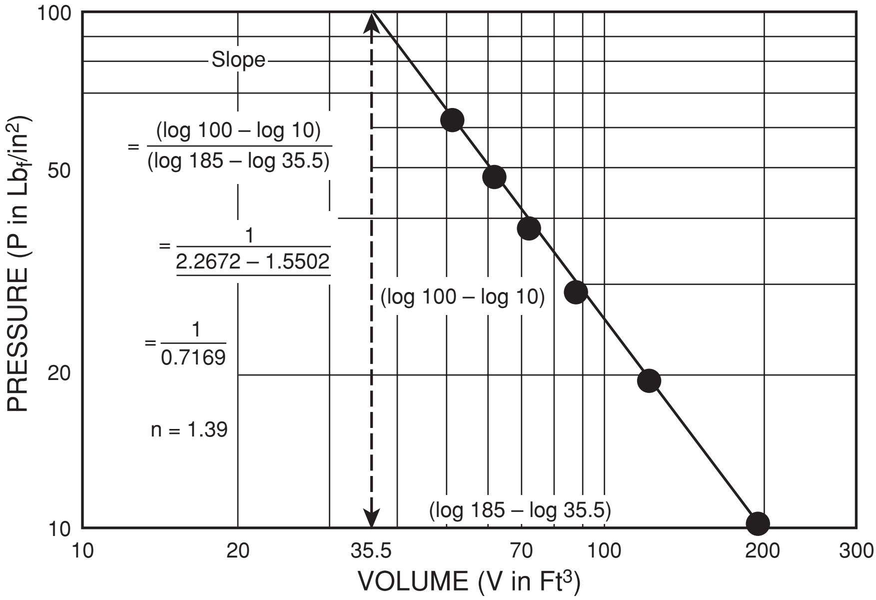

Figure 1.7 Log-log graph of pressure against volume during adiabatic expansion of a gas to determine the adiabatic expansion coefficient from the slope.

Thus, the value of n will be the negative slope of the best-fitting line line drawn through the data points in a log-log graph. The log-log graph of the data is shown in Fig. 1.7. The slope is -1.39, therefore the value of n is 1.39. This problem can be solved using linear regression analysis after transforming the data such that $x = \log(V)$ and $y = \log(P)$. The sums are $\Sigma x = 11.6953$; $\Sigma y = 8.7975$; $\Sigma x^2 = 23.006$; $\Sigma y^2 = 13.3130$; $\Sigma xy = 16.8544$

$$a = \frac{16.8544 - 8.7975(11.6953)/6}{23.006 - (11.6953)^2/6} = -1.40$$

$$b = \frac{8.7975(23.006) - (11.6953)(16.8544)}{6[23.006 - (11.6953)^2/6]} = 4.2033$$

$$r = \frac{6(16.8544) - (11.6953)(8.7975)}{[[6(23.006) - (11.6953)^2][6(8.7975) - (13.3130)^2]]^{0.5}}$$

$r = -0.9986$. r is very close to 1.0, indicating good fit of the data points to the linear regression equation. The value of n equals the slope, therefore, $n = 1.40$

1.5 INTERCEPT OF LOG-LOG GRAPHS

The y-intercept of a log-log graph is determined at a point where $\log x = 0$. On a log-log plot, $\log x = 0$ when $x = 1$. Therefore, the y-intercept is read from the graph at a point where the line crosses $x = 1$. In Example 1.10, log C is the y-intercept of the line. Figure 1.8 is drawn by

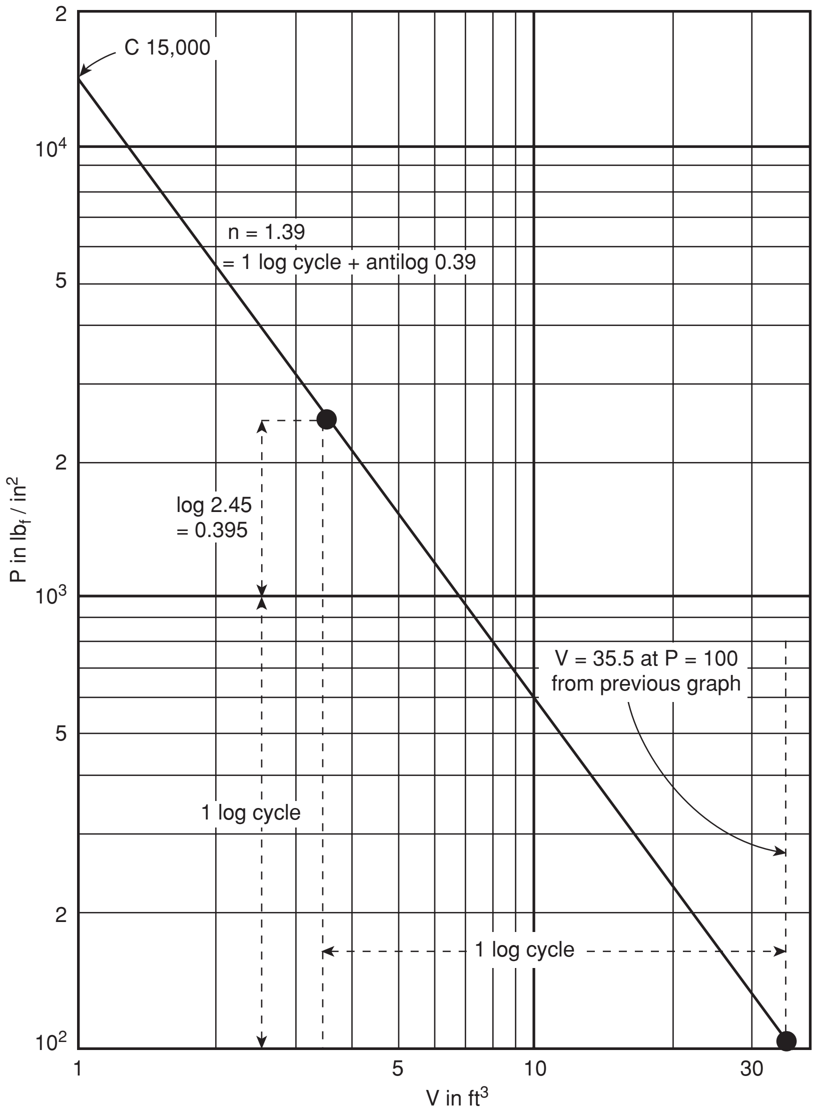

Figure 1.8 Plotting a linear log-log graph based on one point and slope, and intercept of a log-log graph.

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extending the graph in Fig. 1.7 to include V = 1 in order to show how C may be evaluated from the intercept. The line passes through the point V = 35.5 and P = 100.

The slope, 1.39, is used to generate the other point on the line by reducing V one log cycle to a point with coordinate 3.55 and going up 1.39 log cycles; that is, 100 to $1000(10^{0.39})$ or 2450. Thus, the coordinate of the second point is 3.55, 2480. Joining the two points by a straight line and extrapolating the line to V = 1, the value of the intercept, which is 15,000, may be obtained. Thus, C = 15,000. From the regression, the intercept = 4.2033.C = $10^{4.2033}$ = 15,500.

1.6 ROOTS OF EQUATIONS

The roots of an equation $F(x) = 0$ are the points where the function crosses the abscissa. The roots of a system of equations are values of the variables that satisfy the equations and represent a point in the graph where the equations intersect. The following techniques are used to determine roots of equations.

1.6.1 Polynomials

A polynomial expression will have as many roots as the order of the equation. A root may be real or imaginary. Examples of imaginary roots are negative numbers raised to a fractional power. In this book, only real roots will be considered. The following techniques can be used in evaluating roots of polynomials.

1.6.1.1 Quadratic Equation

Equations with 2 as the highest power of the variable are called quadratic equations, and the root is obtained using the quadratic formula. The equation:

$$ax^2 + bx + c = 0$$

will have the following roots:

$$x = \frac{-b \pm \sqrt{(b^2 - 4ac)}}{2a}$$

Example 1.11. Determine the roots of the expression:

$$2x^2 + 3x - 2 = 0$$

Using the quadratic equation, $a = 2$, $b = 3$, $c = -2$

$$x = \frac{-3 \pm \sqrt{(3)^2 - (4)(2)(-2)}}{2(2)}$$

$x = 0.686;\ x = -2.186$

1.6.1.2 Factoring

Equations may be factored and the roots of the individual factors calculated. Thus:

$$F(x) = (ax + b)(cx + d)(ex + f) = 0$$
$$x = -b/a; \qquad x = -d/c; \qquad x = -f/e$$

All three values of x satisfy the equality $F(x) = 0$.

Example 1.12. Determine the roots of the equation: $2x^3 + 5x^2 - 11x + 4 = 0$. Dividing by $2x - 1$, the quotient is $x^2 + 3x - 4$, which when further divided by $x - 1$ will give a quotient of $x + 4$. Thus the factors $(2x - 1)(x - 1)(x + 4) = 2x^3 + 5x^2 - 11x + 4 = 0$. The roots are $x = 1/2$; $x = 1$; and $x = -4$.

1.6.1.3 Iteration Technique

This is a trial-and-error method involving the substitution of values of the variable into the equation and testing if equality expressed by the function is satisfied. Inspection will usually identify a range of values of the variable that gives a negative value for the function at one end of the range and a positive value at the other end. Substitution of values within that range and plotting will identify the value of the variable when the function crosses the abscissa.

Another method for iteration involves the calculus, and is called the Newton-Raphson iteration procedure. In this procedure, a value of the variable (x_1) is assumed and the next value (x_2) can be calculated as follows:

$$x_2 = x_1 - \frac{F(x)}{F'(x)}$$

The iteration is continued until $F(x) = 0.F'(x)$ is the value of first derivative of the function evaluated at the assumed value of x. The derivative is discussed in Section 1.3.

Example 1.13. Determine the roots of the function F(x): $2x^3 + 5x^2 - 11x + 4 = 0$.

This is the same function as the previous example, therefore the results of the iteration method can be verified. Because this is a cubic expression, three roots are to be expected. Using differential calculus, the derivative of the function is determined.

$$F'(x) = 6x^2 + 10x - 11$$

If this derivative is equated to zero, the values of x where the function exhibits a maximum and minimum can be determined. The roots of $6x^2 + 10x - 11 = 0$ can be determined using the quadratic equation as follows:

$$x = \frac{-10 \pm \sqrt{100 - 4(6)(-11)}}{2(6)}; \quad x = -2.432; \quad x = 0.755$$

Because these two points represent a peak and a valley in the curve, it would be expected that one root might exist at $x < -2.423$, one at $-2.423 < x < 0.755$, and another root at $x > 0.755$. To illustrate the Newton-Raphson iterative technique, consider the root at the region $-2.423 < x < 0.755$. First, Let $x = -1$; $F(x) = 18$; $F'(x) = -15$; $x_2 = -1 - 18/(-15) = +0.2$. x_2 is assumed to be the new value of x in the next iteration. Let $x = 0.2$; $F(x) = 2.016$; $F'(x) = -8.76$. $x_2 = 0.2 - (2.016/-8.76) = 0.43$. This is used as the new value of x in the next iteration.

Let $x = 0.43$; $F(x) = 0.353$; $F'(x) = -5.59$:

$$x_2 = 0.43 - \frac{0.0353}{-5.59} = 0.493$$

Using the new value of x in the next iteration: Let x = 0.493; F(x) = 0.032; F'(x) = -4.612:

$$x_2 = 0.492 - \frac{0.032}{-4.612} = 0.4999$$

The iteration is terminated when a critical value of $|x - x_2|$ is reached. For example, if the critical $|x - x_2|$ is 0.0001, another iteration is needed with $x = 0.4999$. $F(x) = 0.00045$; $F'(x) = -4.5016$ and $x_2 = 0.4999 + 0.00045/4.5016$; $x_2 = 0.5000$. Thus, the critical $|x - x_2|$ of 0.0001 is reached and the iteration is stopped. The value of x is the last one computed, which is 0.5000.

The root in this region of the function as shown in the previous example is 0.5. A similar process can be used to determine the other two roots.

1.7 PROGRAMMING USING VISUAL BASIC FOR APPLICATIONS IN MICROSOFT EXCEL

BASIC stands for "Beginner's All-purpose Symbolic Instruction Code." It is a program that interprets symbols and codes and convert them into machine language that the computer can process. The usefulness of BASIC is reinforced by bundling of the Visual BASIC interpreter in one of the more popular spreadsheet programs, Excel. Although spreadsheets may be used to solve equations, there are situations when BASIC is more efficient to use than spreadsheets. Formulas used to calculate values in spreadsheet programs are coded using BASIC syntax. The format of BASIC is very similar to processing a problem manually. The computer executes the commands in sequence. For example, when an iterative procedure is used to solve the function $F(x) = 0$, an estimated value of the variable is substituted into the equation for F(x), F(x) is calculated, and the process is repeated until $F(x) = 0$. The repeated calculations are done rapidly by the computer. The Newton-Raphson iteration technique in BASIC facilitates determining roots of equations. Visual BASIC is the latest version of the language. In Visual BASIC, the program statements are executed consecutively, therefore make sure that variables have been defined and values are known before any variable is used in a program line. Data may be entered using the "*inputbox*" command, by defining values of variables using an equality statement or by using a dimension statement, for example, *Dim* y(i), to enter data as an array. Answers are displayed using the *Msgbox* function. The following example illustrates the use of Visual BASIC in an iterative procedure for determining the root of a function.

Example 1.14. Determine the positive root of the function $x^2 + 109.3x^{1.35} - 20,000 = 0$. The solution is based on substitution of various values of x into the equation. To illustrate Visual BASIC programing, the program inside Microsoft Excel will be used.. Start Excel. From the main menu, access the BASIC interpreter by selecting *View*, then select *Toolbar* in the pop-up menu and select *Visual BASIC* in the secondary menu. The Visual BASIC message box appears. Select the "Visual Basic Editor" icon, which brings up the Visual Basic Main Window. Select *View* and *Code* in the pop-up menu. This opens the Visual BASIC window. The window is now available for coding the program. First type the subject **Sub** and the title of the subject, for example, **Root1**. Pressing the "Enter" key automatically displays "End Sub" in the window. The program code can then be typed in the space between "Sub" and "End Sub." Displays can be formatted by declaring a named variable to be displayed; for example, **Display** = and the variables and values to be displayed. Include the "Chr(10)" and "Chr(13)," the linefeed and return codes, to separate the lines in the display. At the point in the program where the values to be displayed are created, write the code "MsgBox Text." The program and display are shown in Fig. 1.9. The output of the program is as follows:

The first line in the program defines the type (Sub or Function), name and arguments, and is the procedure header. The last line in the program is the procedure footer. These two lines in the program define the procedure's limits in Visual BASIC.

The program is run by clicking on the "Run" icon. The screen will display each set of x and corresponding fx values in one line as defined by the Chr(10), a linefeed code, and Chr(13), a carriage return code, in statement to be printed. The value of x can be set at the beginning from a wider range (e.g., from 1 to 100 in step of 1), then narrowed down to a smaller range to obtain more significant figures in the value of the root.

The values of fx changes from negative (−6.259) at $x = 43.96$ to positive (0.1673) at $x = 43.97$. Thus, the root must be just below and close to 43.97. A more accurate value for the root may be obtained using the Newton-Raphson iteration technique.

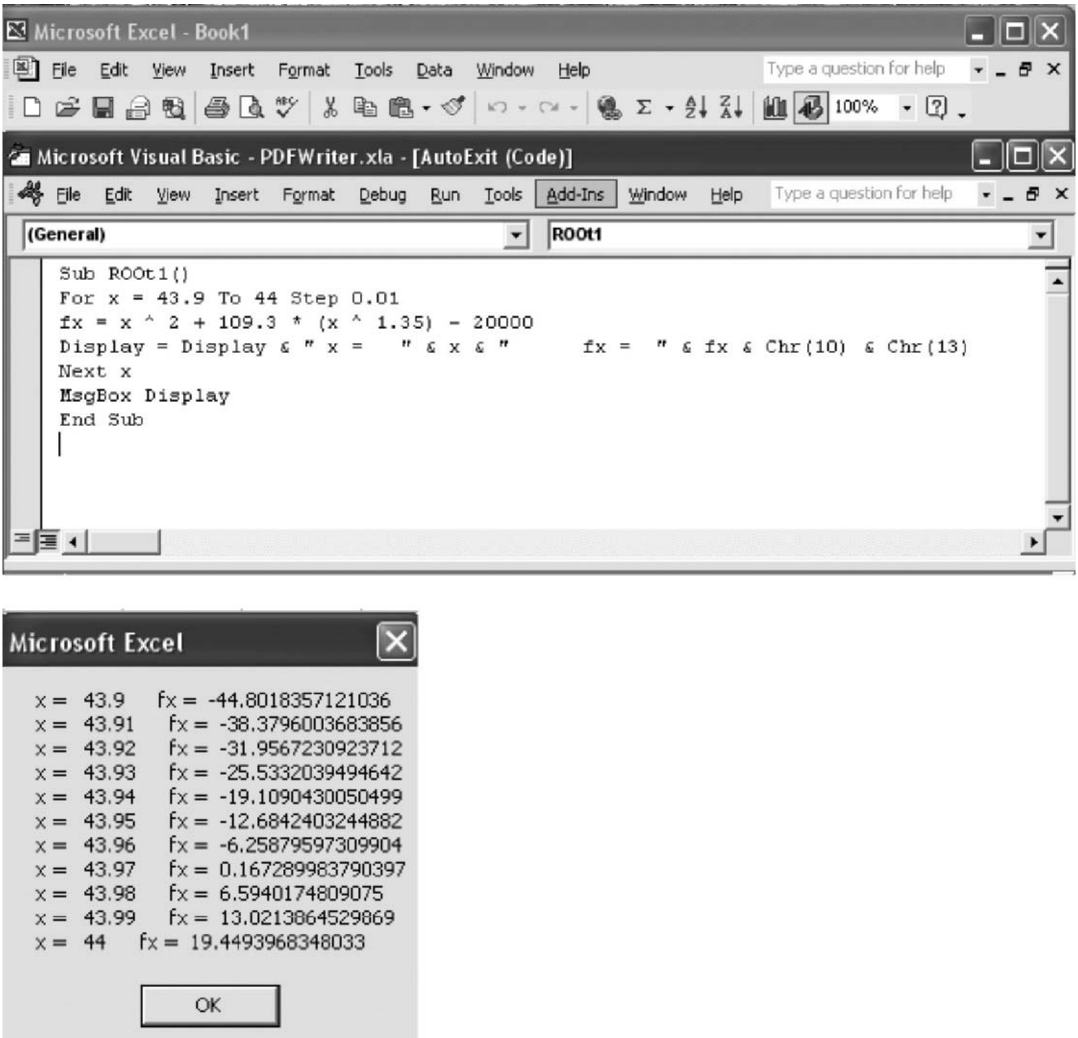


Figure 1.9 Coding of Visual BASIC program for calculating the root of a function and the display on running the program.

Solution:

Using the Newton-Raphson iteration technique, $F = (x) = 2x + 147.555x^{0.35}$.
The Visual BASIC program is shown in Fig. 1.10.
The program, when run, will output x = 43.96973968 as shown in Fig. 1.10.

Note that the message box is displaying only one line and is outside of the loop; there is no need to code the display as a variable as in the previous example.

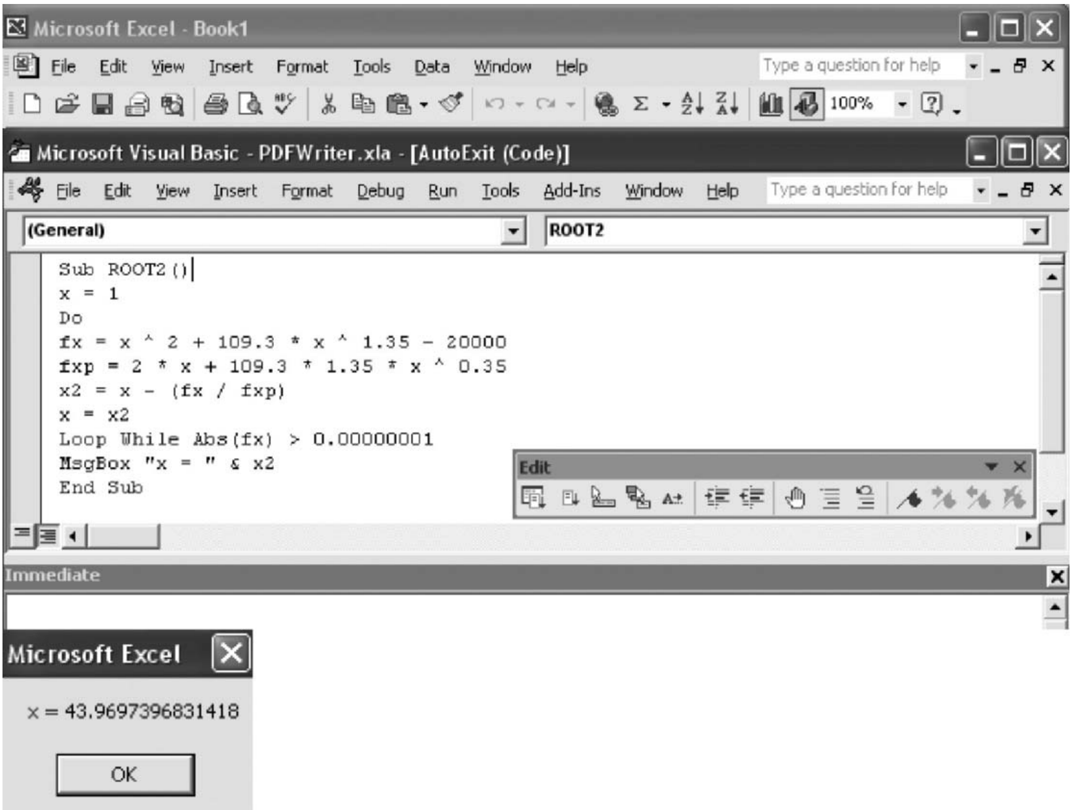


Figure 1.10 Coding of Visual BASIC program for calculating the root of a function using Newton-Raphson iteration and the display on running the program.

1.8 USE OF SPREADSHEETS TO SOLVE ENGINEERING PROBLEMS

There are three major spreadsheet programs available: Excel, Quatro Pro, and Lotus 1, 2, 3. Although there are similarities in navigating within the spreadsheet and programming formulas in cells, there are differences in syntax, therefore it is best to study one particular software rather than switch around among the different types. Excel will be used to demonstrate the concepts. Each cell in the spreadsheet may be filled by typing a title or a number. Values calculated using a formula can also be entered. *Formulas* are created with the syntax of BASIC, which are as follows:

Multiplication: $xy = x*y$ Logarithms: $\log_{10} x = \log(x); \log_e x = \ln(x)$
Division: $x\ )\ y = x/y$ Exponentiation: $x^a = x\wedge a$

To *navigate between cells*, use the arrow keys. *Correcting entries in cells* may be done by typing a new entry completely inside a cell. Moving cursor to another cell will replace old content in a cell with new one. An alternative is to press F2, correct part of the contents of a cell, and press "Enter."

Copying formulas form one cell to other cells is done by locating the cursor on the cell to be copied, left clicking on the "copy" icon, and dragging the mouse to range of cells where you want the cell content to be copied. Then left click on the "paste" icon to complete the entry into the other cells. When copying contents of one cell to be used on all calculations in the block of cells to which a formula is copied, make sure to use the *absolute addressing* method. This is done by placing the $ sign before the column and row designation for a cell. Thus, if the value is in C2, an absolute cell address would be $C$2. Values in either column or row may be frozen. For example, values in column A from row 1 to 20 will be used in a formula in column D, E, and F. The cell address may be written as $C1, $C2, and so forth, in either column D, E, or F, and values from column C will always be used in the calculation. On the other hand, if relative addressing is used, and formulas in column D are copied to column E, there will be an error because the column E formulas will be using values in column D instead of column C. Thus addressing a cell as $A$2 means that the content of cell A2 will be used in all formulas regardless of location in the spreadsheet. Using the cell address $A2 means that the contents of cells in column A will be used in the calculations regardless of the column position in the spreadsheet. When *entering formulas*, use the = sign before starting the formula to tell the program to treat the entry as a formula rather than a label. When using formula calculated values in cells in another formula, an error message may be returned because the cell addresses may no longer be compatible with the current cell position in the spreadsheet. This may be corrected by absolute addressing or by *converting formula value in cells to numerical values*. To change formula values in a cell to a numerical value, position the cursor in the cell, double click, press F9 and enter.

Example 1.15. Calculate the root of the following equation by iteration using the Newton-Raphson iteration technique: $Y = X^2 + 109.3\ X^{1.35} - 20{,}000$.

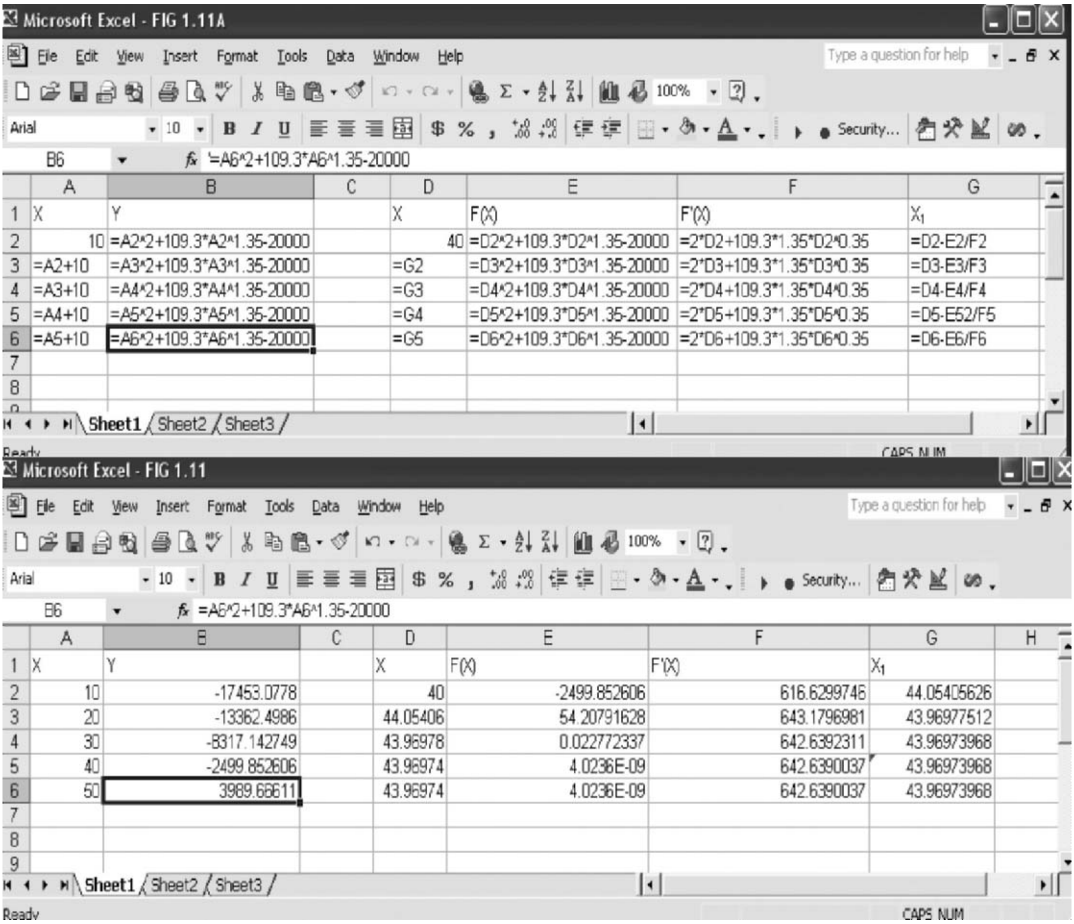
Solution:

Newton-Raphson is discussed in the preceding section.

The function is F(x) = x^2 + 109.3*x^1.35 − 20,000.
The first derivative is F = (x) = 2*X + 109.3*1.35*x^.35.
Start Excel. To determine an approximate value for x when y = 0, start with fairly large increments of x and calculate values for y. Label cell A1, x, and cell B1, y. Enter 10 in A2 and enter formula = A2 + 10 in A3. Copy formula in A3 to A4 to A6. Enter the formula = x^2 + 109.3*x^1.35 − 20000 in B2. Copy the formula in B2 to B3 to B6. Note that y changes from negative to positive between x = 40 and x = 50. Start Newton-Raphson with an initial value of x = 40.
In the spreadsheet D1, E1, F1 and G1, enter the labels X, F(x), and F = (x), X2.
In D2, enter a starting value of X , 40.
In E2, enter the formula = D2^2 + 109.3*D2^1.35 − 20000.
In F2, enter the formula = 2*D2 + 109.3*1.35*D2^.35.
In G2, enter the formula = D2 − (E2/F2).
In D3, enter (calculated value of x2) formula = $G2.
Copy formula in D3 to D4 to D6, and also corresponding formulas in columns E, F, and G. The value of x that gives 0 for the value of F(x) is the root. This value is 43.9674. The spreadsheet is shown in Fig. 1.11.

Example 1.16. Calculate the moisture content needed to lower the water activity of a gelatin candy to 0.7. The candy contains 7.5 g gelatin/40 g dextrose. The water activity a_w changes with mole fraction water, x , according to:

$$\log_{10}\left(\frac{a_w}{x}\right) = -0.7(1-x)^2$$



	A	B	C	D	E	F	G
1	X	Y		X	F(X)	F'(X)	X_1
2	10	=A2^2+109.3*A2^1.35-20000		40	=D2^2+109.3*D2^1.35-20000	=2*D2+109.3*1.35*D2^0.35	=D2-E2/F2
3	=A2+10	=A3^2+109.3*A3^1.35-20000		=G2	=D3^2+109.3*D3^1.35-20000	=2*D3+109.3*1.35*D3^0.35	=D3-E3/F3
4	=A3+10	=A4^2+109.3*A4^1.35-20000		=G3	=D4^2+109.3*D4^1.35-20000	=2*D4+109.3*1.35*D4^0.35	=D4-E4/F4
5	=A4+10	=A5^2+109.3*A5^1.35-20000		=G4	=D5^2+109.3*D5^1.35-20000	=2*D5+109.3*1.35*D5^0.35	=D5-E52/F5
6	=A5+10	=A6^2+109.3*A6^1.35-20000		=G5	=D6^2+109.3*D6^1.35-20000	=2*D6+109.3*1.35*D6^0.35	=D6-E6/F6

	A	B	C	D	E	F	G
1	X	Y		X	F(X)	F'(X)	X_1
2	10	-17453.0778		40	-2499.852606	616.6299746	44.05405626
3	20	-13362.4986		44.05406	54.20791628	643.1796981	43.96977512
4	30	-8317.142749		43.96978	0.022772337	642.6392311	43.96973968
5	40	-2499.852606		43.96974	4.0236E-09	642.6390037	43.96973968
6	50	3989.66611		43.96974	4.0236E-09	642.6390037	43.96973968

Figure 1.11 Spreadsheet solution to root of an equation using Newton-Raphson iteration.

Solution:

Use as a basis 47.5 g gelatin/dextrose mixture (7.5 g gelatin; 40 g dextrose). Let M be the mass fraction moisture in candy. The mass of water = 47.5/(1 − M) − 47.5 = 47.5M/(1 − M). The mole fraction of water (x) at mass fraction water M is

$$x = \frac{\dfrac{47.5M}{18(1-M)}}{\dfrac{47.5M}{18(1-M)} + \dfrac{40}{180}}$$

Label cell A1, M; B1, x; and C1, aw. In A2, enter M = 0.9; in A3, enter = A2 − 0.1. Copy to A4:A10. In B2, enter formula = (47.5*A2/(18*(1 − A2))) /((47.5*A2/(18*(1 − A2))) + 40/180). Copy to B3:B10. In C2, enter formula = B2*10^(−.7*(1 − B2)^2). Copy to C3:C10. Inspection of the calculated values show that M should be close to 0.3. Replace value in A2 with 0.25 and decrement by 0.01 to A6. Recalculated values show M to be between 0.21 and 0.22 for $a_w = 0.7$. Thus, the candy formula should have a moisture content greater than 21% but less than 22%. The spreadsheet is shown in Fig. 1.12.

1.9 SIMULTANEOUS EQUATIONS

Simultaneous equations are often encountered in problems involving material balances and multistage processes. The following techniques are used in evaluating simultaneous equations.

1.9.1 Substitution

If an expression for one of the variables is fairly simple, substitution is the easiest means of solving simultaneous equations. In a set of equations $x + 2y = 5$ and $2x - 2y = 3$, x may be expressed as a function of y in one equation and substituted into the other to yield an equation with a single unknown. Thus, $x = 5 - 2y$ and $2(5 - 2y) - 2y = 3$, giving a value of $y = 7/6$, and $x = 8/3$.

1.9.2 Elimination

Variables may be eliminated either by subtraction or division. Division is used usually with geometric expressions, and elimination by subtraction is used with linear expressions. When subtraction is used, equations are multiplied by a factor such that the variable to be eliminated will have the same coefficient in two equations. Subtraction will then yield an equation having one less variable than the original two equations.

Example 1.17. Calculate the value of τ and μ that would satisfy the following expressions: $\mu = 3.2\ (\tau)^{0.75}$ and $1.5\mu = 0.35(\tau)^{0.35}$.

μ is eliminated by division.

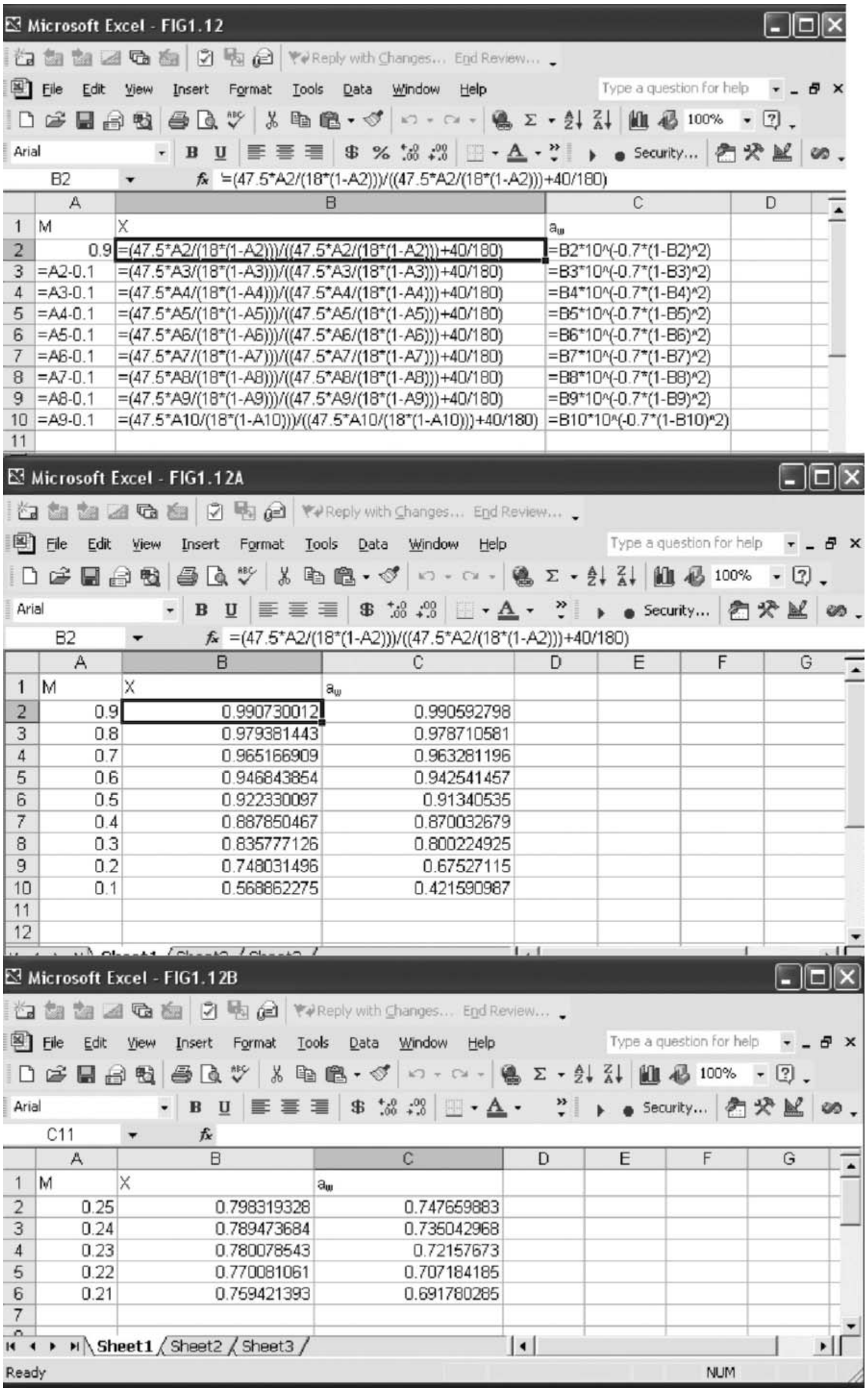
$$\frac{1}{1.5} = \frac{3.2}{0.35}\tau^{0.75-0.35}$$
$$\tau = \frac{0.35}{(1.5)(3.2)}\frac{1}{0.4}$$

$$\tau = 0.00169; \quad \Phi = 3.2(0.00169)^{0.75} = 0.02667$$

Example 1.18. Determine x and y that satisfy the following expressions: $2x + 2y = 32$; $x^2 = y - 2$.

y may be eliminated by multiplying the second equation by 2 and adding the two equations.

$$2x + 2y = 32$$
$$2x^2 - 2y = -4$$



Microsoft Excel - FIG1.12

B2 f_x =(47.5*A2/(18*(1-A2)))/((47.5*A2/(18*(1-A2)))+40/180)

	A	B	C	D
1	M	X	a_w	
2	0.9	=(47.5*A2/(18*(1-A2)))/((47.5*A2/(18*(1-A2)))+40/180)	=B2*10^(-0.7*(1-B2)^2)	
3	=A2-0.1	=(47.5*A3/(18*(1-A3)))/((47.5*A3/(18*(1-A3)))+40/180)	=B3*10^(-0.7*(1-B3)^2)	
4	=A3-0.1	=(47.5*A4/(18*(1-A4)))/((47.5*A4/(18*(1-A4)))+40/180)	=B4*10^(-0.7*(1-B4)^2)	
5	=A4-0.1	=(47.5*A5/(18*(1-A5)))/((47.5*A5/(18*(1-A5)))+40/180)	=B5*10^(-0.7*(1-B5)^2)	
6	=A5-0.1	=(47.5*A6/(18*(1-A6)))/((47.5*A6/(18*(1-A6)))+40/180)	=B6*10^(-0.7*(1-B6)^2)	
7	=A6-0.1	=(47.5*A7/(18*(1-A7)))/((47.5*A7/(18*(1-A7)))+40/180)	=B7*10^(-0.7*(1-B7)^2)	
8	=A7-0.1	=(47.5*A8/(18*(1-A8)))/((47.5*A8/(18*(1-A8)))+40/180)	=B8*10^(-0.7*(1-B8)^2)	
9	=A8-0.1	=(47.5*A9/(18*(1-A9)))/((47.5*A9/(18*(1-A9)))+40/180)	=B9*10^(-0.7*(1-B9)^2)	
10	=A9-0.1	=(47.5*A10/(18*(1-A10)))/((47.5*A10/(18*(1-A10)))+40/180)	=B10*10^(-0.7*(1-B10)^2)	
11				

Microsoft Excel - FIG1.12A

B2 f_x =(47.5*A2/(18*(1-A2)))/((47.5*A2/(18*(1-A2)))+40/180)

	A	B	C
1	M	X	a_w
2	0.9	0.990730012	0.990592798
3	0.8	0.979381443	0.978710581
4	0.7	0.965166909	0.963281196
5	0.6	0.946843854	0.942541457
6	0.5	0.922330097	0.91340535
7	0.4	0.887850467	0.870032679
8	0.3	0.835777126	0.800224925
9	0.2	0.748031496	0.67527115
10	0.1	0.568862275	0.421590987
11			
12			

Microsoft Excel - FIG1.12B

C11 f_x

	A	B	C
1	M	X	a_w
2	0.25	0.798319328	0.747659883
3	0.24	0.789473684	0.735042968
4	0.23	0.780078543	0.72157673
5	0.22	0.770081061	0.707184185
6	0.21	0.759421393	0.691780285
7			

Sheet1 / Sheet2 / Sheet3

Ready NUM

Figure 1.12 Spreadsheet solution to problem of candy moisture content to give a water activity of 0.70.

Adding: $\quad 2x^2 + 2x = 28$

$$x = \frac{-2 \pm \sqrt{4 - 4(2)(-28)}}{2(2)}$$

Solving by the quadratic formula:
$x = 3.275; \quad y = 12.275$
$x = -4.275; \quad y = 20.275$

1.9.3 Determinants

Coefficients of a system of linear equations may be set up in an array or matrix, and the matrices are resolved to determine the values of the variables. Solutions of a system of linear equations may be obtained using a spreadsheet program like Excel. For a system of three equations or more, setting up the matrix to solve the equations using Excel will be the fastest way to determine the values of the variables.

In a system of equations:

$$a_1x + b_1y + c_1z = d_1$$
$$a_2x + b_2y + c_2z = d_2$$
$$a_3x + b_3y + c_3z = d_3$$

the array of the coefficients is as follows:

$$\begin{array}{llll} |a_1 & b_1 & c_1| & |d_1| \\ |a_2 & b_2 & c_3| & |d_2| \\ |a_3 & b_2 & c_3| & |d_3| \end{array}$$

The values of x, y, and z are determined as follows:

$$x = \frac{\begin{bmatrix} d_1 & b_1 & c_1 \\ d_2 & b_2 & c_2 \\ d_3 & b_3 & c_3 \end{bmatrix}}{\begin{bmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{bmatrix}} \qquad y = \frac{\begin{bmatrix} a_1 & d_1 & c_1 \\ a_2 & d_2 & c_2 \\ a_3 & d_3 & c_3 \end{bmatrix}}{\begin{bmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_2 & c_3 \end{bmatrix}} \qquad z = \frac{\begin{bmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{bmatrix}}{\begin{bmatrix} a_1 & b_1 & c_1 \\ a_2 & b_2 & c_2 \\ a_3 & b_3 & c_3 \end{bmatrix}}$$

A 2×2 matrix is resolved by cross-multiplying the elements in the array and subtracting one from the other. The position of an element in the matrix is designated by a subscript ij with i representing the row and j representing the column. In order to maintain consistency in the sign of the cross-product, the element in the first column whose subscript adds up to an odd number is assigned a negative sign. Thus, the cross-product with that element will have a negative sign.

A 2×2 matrix and its value is shown below:

$$\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = a_{11}a_{22} - a_{21}a_{12}$$

A 3×3 matrix is evaluated by multiplying each of the elements in the first column with the 2×2 matrix left using elements in the second and third column other than those in the same row as the multiplier. As with the 2×2 matrix above, the multiplier whose subscript adds up to an odd number is assigned a negative value. The multiplier and 2×2 matrices as multiplicand are determined as follows:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

Thus, the 3×3 matrix resolves into:

$$a_{11} \begin{bmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{bmatrix} - a_{21} \begin{bmatrix} a_{12} & a_{13} \\ a_{32} & a_{33} \end{bmatrix} + a_{31} \begin{bmatrix} a_{12} & a_{13} \\ a_{22} & a_{23} \end{bmatrix}$$

Example 1.19. Determine the values of x, y, and z in the following equations:

$$x + y + z = 100$$
$$0.8x + 0.62y + z = 65$$
$$0.89x + 0.14y = 20$$

The array of the coefficients and constants is as follows:

$$\begin{bmatrix} 1 & 1 & 1 \\ 0.8 & 0.62 & 1 \\ 0.89 & 0.14 & 0 \end{bmatrix} \begin{bmatrix} 100 \\ 65 \\ 20 \end{bmatrix}$$

The matrix (array A) that consists of the coefficients of the variables will be the denominator of the three equations for x, y, and z.

$$\begin{bmatrix} 1 & 1 & 1 \\ 0.8 & 0.62 & 1 \\ 0.89 & 0.14 & 0 \end{bmatrix} = 1 \begin{bmatrix} 0.62 & 1 \\ 0.14 & 0 \end{bmatrix} - 0.8 \begin{bmatrix} 1 & 1 \\ 0.14 & 0 \end{bmatrix} + 0.89 \begin{bmatrix} 1 & 1 \\ 0.62 & 1 \end{bmatrix}$$
$$= 1(0 - 0.14) - 0.8(0 - 0.14) + 0.89(1 - 0.62)$$
$$= 0.3102$$

The matrix (array B) that will be the numerator in the equation for x is

$$\begin{bmatrix} 100 & 1 & 1 \\ 65 & 0.62 & 1 \\ 20 & 0.14 & 0 \end{bmatrix} = 100 \begin{bmatrix} 0.62 & 1 \\ 0.14 & 0 \end{bmatrix} - 65 \begin{bmatrix} 1 & 1 \\ 0.14 & 0 \end{bmatrix} + 20 \begin{bmatrix} 1 & 1 \\ 0.62 & 1 \end{bmatrix}$$
$$= 100(0 - .14) - 65(0 - .14) + 20(1 - .62) = 2.7$$

Thus, $x = 2.7/.3102 = 8.7$.

The matrix (array C) that is the numerator in the equation for y is

$$\begin{bmatrix} 1 & 100 & 1 \\ 0.8 & 65 & 1 \\ 0.89 & 20 & 0 \end{bmatrix} = 1 \begin{bmatrix} 65 & 1 \\ 20 & 0 \end{bmatrix} - 0.8 \begin{bmatrix} 100 & 1 \\ 20 & 0 \end{bmatrix} + 0.89 \begin{bmatrix} 100 & 1 \\ 65 & 1 \end{bmatrix}$$
$$= 1(0 - 20) - 0.8(0 - 20) + 0.89(100 - 65) = 27.15$$

Thus, $y = 27.15/0.3102 = 87.5$.

The matrix (array D) that is the numerator of the equation for z is

$$\begin{bmatrix} 1 & 1 & 100 \\ 0.8 & 0.62 & 65 \\ 0.89 & 0.14 & 20 \end{bmatrix} = 1\begin{bmatrix} 0.62 & 65 \\ 0.14 & 20 \end{bmatrix} - 0.8\begin{bmatrix} 1 & 100 \\ 0.14 & 20 \end{bmatrix} + 0.89\begin{bmatrix} 1 & 100 \\ 0.62 & 65 \end{bmatrix}$$

$$= 1(12.4 - 9.1) - 0.8(20 - 14) + 0.89(65 - 62) = 1.17$$

Thus, $z = 1.17/0.3102 = 3.8$.

Check: $x + y + z = 8.7 + 87.5 + 3.8 = 100$.

Values of determinants may be obtained using Microsoft Excel. Determinants of arrays A, B, and C above will be solved. Access Excel and enter the arrays A, B, C, and D above. For example, the array A may be entered in the block A2 to C4, array B in block E2 to G4, array C in block A8 to C10, and array D in block E8 to G10. To determine determinant of array A, block A2 to C4, move the pointer to the name box (displaying "A2") and give the array a name (e.g., ARRA). Press "Enter." Move the pointer to the cell where the answer is to be displayed (e.g., B5 for array A) and click the mouse to make B5 the active cell. Move the pointer to the formula box and click on the "=" sign. This activates the formula box. Type "Mdeterm(ARRA)" and select *OK*. The determinant of array A (.3102) will be displayed in cell B5. Repeat the process for arrays B, C, and D. Figure 1.13 shows the spreadsheet. The results are exactly the same as those solved manually above.

1.10 SOLUTIONS TO A SYSTEM OF LINEAR EQUATIONS USING THE "SOLVER" MACRO IN EXCEL

Instead of calculating determinants, solutions to a system of equations may be obtained by using the "Solver" macro in Excel. Enter the variables = coefficients into the spreadsheet as an array. Enter the row of constants in the row adjacent to the array of variables = coefficients. Then select a row of cells where the answer will be displayed. This can be the empty row above or below the array. Enter zero in each of these cells. Enter the constraints in an empty column to the right of the array. The constraints will be formulas equivalent to the equations to be solved. Position the pointer in the cell to contain the first constraint, click to make this the active cell, move the pointer to the formula box, and click on the "=" sign. This activates the formula box. Enter the formula in this cell. Use absolute cell addressing for the cells designated to contain the values of the variables. Enter all constraints. Excel will enter zero in these constraints cells when the formulas are entered. Select *Tools* then select *Solver* in the pop-up menu. The *Solver Parameters* dialogue box displays. Point the mouse to the first cell containing the constraint. This cell address will be displayed in the *Set Target Cell* box. Click *Value of* and enter the value corresponding to the constant of the first equation. Click the box under *By Changing Cells* and enter range of cell addresses of the row designated to contain values of the variables. Under *Subject to Constraints* is a box that should hold all the other constraints. Click on *Add* to enter the *Add Constraint* dialogue box. Enter the cell reference for the second constraint formula. Click on the button for the mathematical relationship of the constraint, choose "A=" and click on the box under *Constraint.* Enter the value of the second constant or enter a cell address where this constant was entered. Click *Add.* The *Add Constraint* dialogue box will reappear to accept addition of more constraints. Enter the rest of the constraints. Click *OK*. The *Solver Parameters* dialogue box reappears. Check the values and cell references entered. Click *Solve* and the calculated values of the variables will be displayed in the designated cells.

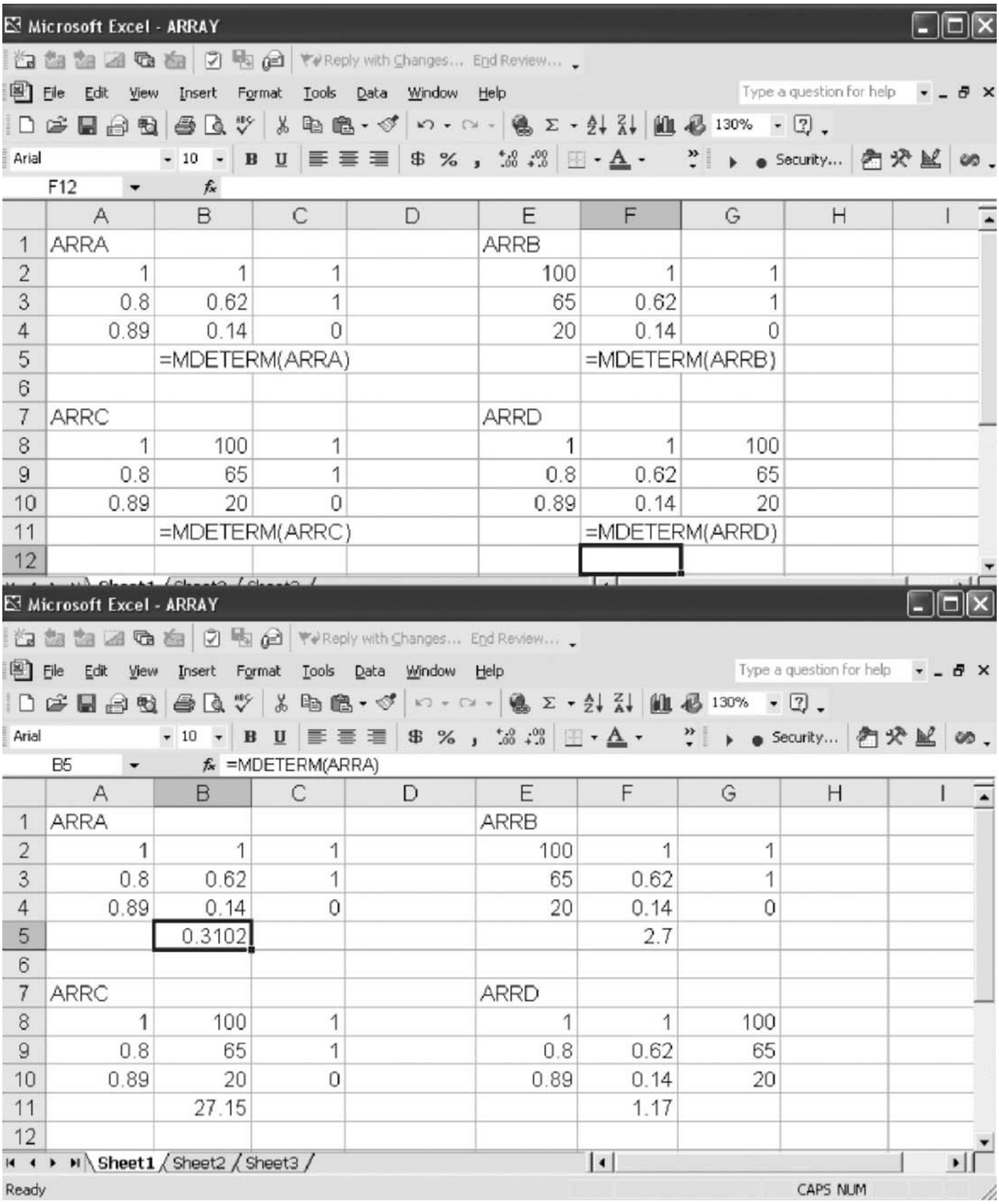


Figure 1.13 Spreadsheet solution to values of determinants using the "Mdeterm" function in Excel.

Example 1.20. Solve the system of equations in the preceding example using the "Solver" macro in Excel.

Solution:

Use the spreadsheet used for calculating determinants above. Enter the array of variables = coefficients in the block A3 to C5. Values for x, y, and z are designated to be displayed in row A8:C8. Enter the constants in column D3:D5. Enter the constraints into the column E3:E5. E3 should have the equivalent of the first equation: Cell $A$8 represents x; $B$8 represents y; and $C$8 represents z. Point the mouse to Cell E3 and click to make it the active cell. Move the pointer to the formula box and Click the "=" sign. Enter the first constraint $A$8*A3 + $B$8*B3 + $C$8*C3. Make cell E4 the active cell, activate the formula box, and enter the second constraint: $A$8*A4 + $B$8*B4 + $C$8*C4. Activate cell E5 and the formula box and enter the third constraint: $A$8*A5 + $B$8*B5 + $C$8*C5. Select *Tools* then *Solver* in the pop-up menu to open the *Solver Parameters* dialogue box. Enter $E$3 for the *Target Cell,* click on *Value of,* and enter the constant of the first equation 100. In the *By Changing Cell* box, enter $A$8:$C$8. In the *Subject to Constraints* box, enter the other constraints by clicking the *Add* button to display the *Add Constraints* dialogue box and enter the *Cell Reference* box $E$4, activate the "=" sign, and enter in the *Constraint* box the cell reference for the second equation constant, $D$4. Click *Add*. The *Add Constraints* dialogue box reappears and enter $E$5, and $D$5. Click *OK*. The *Solver Parameters* dialogue box reappears. Click *Solve*. Results are displayed in Fig. 1.14.

1.11 POWER FUNCTIONS AND EXPONENTIAL FUNCTIONS

Power functions and exponential functions consist of a base raised to an exponent. Although the two functions are similar, "power functions" are those that have numerical exponents, whereas the term "exponential function" is used for those that have variables as exponent. Both functions are resolved using logarithms or by taking the γth root of both sides of the equation, where r is the exponent of the variable whose value needs to be determined. The following are basic rules when working with exponents:

Multiplication: When the base is the same, add exponents

$$x^2(x^3) = x^{2+3} = x^5$$

Division: When the base is the same, subtract exponents. A negative exponent signifies division.

$$\frac{(x+2)^3}{(x+2)^{1.5}} = (x+2)^{3-1.5} = (x+2)^{1.5}$$

Exponentiation: Multiply the exponents. Extracting the γth root of a function implies exponentiation to the $1/\gamma$th power.

$$\left(\frac{P}{V}\right)^{3.5} = P^{3.5}V^{-3.5}$$

$$(x^2)^3 = x^{2(3)} = x^6$$

$$^4\%(x^2) = (x^2)^{1/4} = (x)^{2/4} = (x)^{1/2}$$

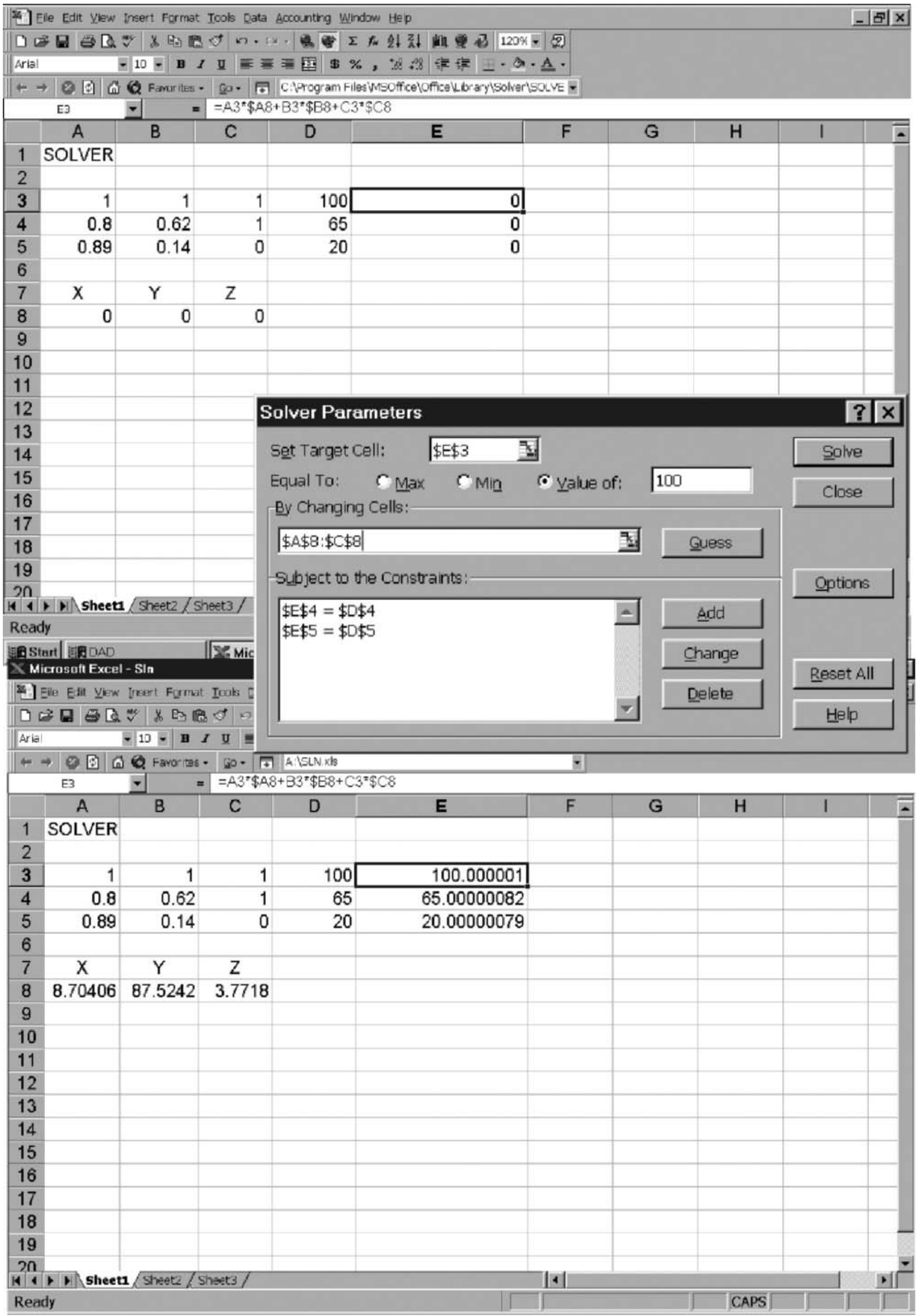


Figure 1.14 Solutions to a system of linear equations using the “Solver” macro in Excel.

1.12 LOGARITHMIC FUNCTIONS

1. Logarithm of a product = sum of the logarithms

   $$\log(xy) = \log x + \log y$$

2. Logarithm of a quotient = difference of the logarithms. A negative logarithm signifies a reciprocal of the terms within the logarithm.

   $$\log(x/y) = \log x - \log\ y$$
   $$-\log x \ \ = \log(1/x)$$

3. Logarithm of a power function = exponent multiplied by the logarithm of the base.

   $$\log e^{2x} = 2x \log e$$

Example 1.21. The Reynolds number of a non-Newtonian fluid is expressed as:

$$\mathrm{Re} = \frac{8V^{2-n}R^n\rho}{k\left(\dfrac{3n+1}{n}\right)^n}$$

Calculate the value of the velocity V that would result in a Reynolds number of 2000 if $k = 1.5$ $\mathrm{Pa \cdot s^n}$, $n = 0.775$, $\rho = 1030\ \mathrm{kg/m^3}$, and $R = 0.0178$ m.

Substituting values:

$$2000 = \frac{8(V)^{1.225}(0.0178)^{0.775}(1030)}{1.5\left[\dfrac{2.325}{0.775}\right]^{0.775}}$$

$$V^{1.225} = \frac{2000(1.5)(2.3429)}{8(0.04406)(1030)} = 25.55$$

$$V = (25.55)^{1/1.225} = 14.08\ \mathrm{m/s}$$

Example 1.22. The temperature (T, in EC) of a fluid flowing through a tube immersed in a constant temperature water bath at T_b changes exponentially with position along the length of the tube as follows:

$$T = T_b - (T_b - T_o)(e)^{-3.425L}$$

Calculate the length L such that when fluid enters the tube with an initial temperature $T_O = 20$ EC, the exit temperature will be 99% of the water bath temperature, T_b, which is 95 EC.

$$T = 0.99(95) = 95 - (95 - 20)(e)^{-3.425L}$$
$$(e)^{-3.425L} = [(95 - 94.05)/(75)] = .012667$$

Taking the natural logarithm of both sides and noting that ln (e) = 1:

$$-3.425L = \ln(.012667); \quad L = -4.3687/-3.425 = 1.276\ \mathrm{m}$$

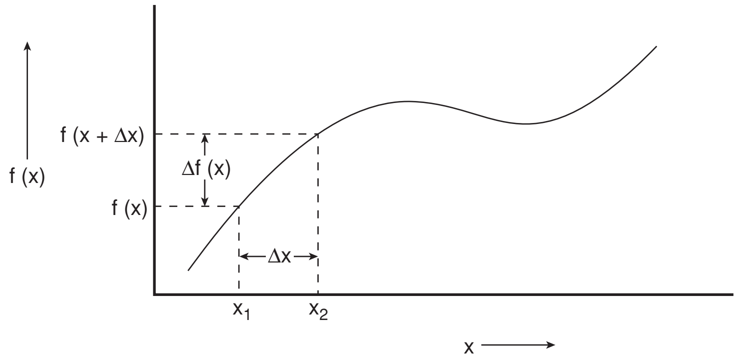


Figure 1.15 Graphical representation of the slope of a function and the derivative.

1.13 DIFFERENTIAL CALCULUS

Calculus is a branch of mathematics that deals with infinitesimal-sized segments of a whole. The concept is analogous to high-speed filming of a moving object. The action can be frozen in an infinitesimal time increment, and it will be possible to take measurements on the frozen picture frame. Analysis of a series of frames will define the nature and magnitude of changes that occur as the object moves. The calculus is particularly useful in predicting point values of variables in a system from global measurements.

Calculus is divided into differential and integral calculus. The former deals with the rate of change of variables or incremental changes in a variable. Integral calculus had its origins on earlier studies of areas of plane figures. An application of integral calculus that is particularly useful to engineers is the derivation of a function that defines a variable or processing parameter from a differential expression of the changes in the variable with respect to another.

1.13.1 Definition of a Derivative

Any function F(x) may be represented by a graph shown in Fig. 1.15. A section on the x axis between x_1 and x_2 is designated Δx. The slope of the function within this section is

$$\text{Slope} = \frac{\Delta F(x)}{\Delta x} = \frac{F(x + \Delta x) - F(x)}{\Delta x}$$

If Δx is infinitesimal, Δx approaches 0, and $\Delta F(x)/\Delta x$ is the derivative of F(x) with respect to x.

$$\underset{\Delta x \to 0}{\text{Limit}} \frac{\Delta F(x)}{\Delta x} = \frac{dF(x)}{dx} = \underset{\Delta x \to 0}{\text{limit}} \frac{F(x + \Delta x) - F(x)}{\Delta x}$$

If the function $F(x) = x^2$:

$$\frac{dF(x)}{dx} = \underset{\Delta x \to 0}{\text{limit}} \frac{(x + \Delta x)^2 - x^2}{\Delta x}$$

$$= \underset{\Delta x \to 0}{\text{limit}} \frac{x^2 + 2x\Delta x + (\Delta x^2) - x^2}{\Delta x}$$

The derivative of $F(x) = x^2$ is $dF(x)/dx = 2x$.
The differential form of the above derivative is

$$dF(x) = 2xdx$$

The symbol "d" is a differential operator, meaning that a differentiation operation has been performed on F(x). Differentiation is the process of obtaining a derivative. The result of a differentiation operation is a differential equation that can then be divided by the differential term of the reference variable to obtain the derivative. The term $dF(x)/dx$ may be written as $F = (x)$.

The derivative is a rate of change, or the slope of a function. Thus, constants will have zero slope and therefore will have a derivative from zero. A linear function will have a constant slope; therefore, the derivative of a variable to the power 1 will be a constant, the coefficient of that variable.

1.13.2 Differentiation Formulas

The following are differentiation formulas that are most often used:

Constant: $d(a) = 0$
Sum: $d[F(x) + G(x)] = dF(x) + dG(x)$
Product: $d[F(x)G(x)] = F(x)dG(x) + G(x)dF(x)$
Quotient: $d(F(x)/G(x)) = (G(x)dF(x) - F(x)dG(x))/[G(x)]^2$
Power function: $d[F(x)]^n = n[F(x)]^{n-1}dF(x)$
Exponential function: $d(a)^{F(x)} = (a)^{F(x)}[dF(x)] \ln a$
Logarithmic function: $d \ln[F(x)] = dF(x)/F(x)$

$D \log[F(x) = dF(x)/F(x)(\ln 10)$

Example 1.23. Determine the slope of the function

$$y = 2(x + 2)^3 + 2x^2 + x + 3$$

at $x = 1$.

The slope is the derivative of the function. The slope is obtained by differentiating the function and solving for dy/dx. The sum and power function formulas will be used.

$$dy = d[2(x + 2)^2] + d(2x)^2 + d(x) + d(3)$$

The last term is the derivative of a constant and is 0.

$$dy = 2(3)(x + 2)^2 d(x + 2) + 2(2)(x)dx + dx = 6(x + 2)^2 dx + 4xdx + dx$$

$$\frac{dy}{dx} = 6(x + 2)^2 + 4x + 1$$

Substituting $x = 1$:

$$\frac{dy}{dx} = 6(3)^2 + 4 + 1 = 54 + 5 = 59$$

Example 1.24. Differentiate the function $H = E + PV$. All terms are variables. Use the sum and the product formulas $dH = dE + PdV + VdP$.

Example 1.25. The expression for the water activity of a sugar solution is given as:
For glucose, k = −0.7. How much faster will the water activity (a_w) change with a change in

$$\log\left[\frac{a_w}{x}\right] = k(1-x)^2$$

water mole fraction (x) at x = 0.7 compared with x = 0.9?

The problem requires determining da_w/dx at x = 0.7 and at x = 0.9. The ratio of the two slopes will give the relative effects of small increases in concentration around x = 0.9 and x = 0.7 on the water activity.

The expression to be differentiated after substituting k = 0.7 is

$$\log\ a_w - \log\ x = -0.7(1-x)^2$$

When differentiated directly in this form, a_w will appear in the denominator of the first term involving $d(\log a_w)$. This can be eliminated by solving first for a_w before differentiation:

$$a_w = x(10)^{-0.7(1-x)^2}$$

Differentiating:

$$\begin{aligned}
d(a_w) &= x d[10]^{-0.7(1-x)^2} + [10]^{-0.7(1-x)^2} dx + [10]^{-0.7(1-x)^2}\ dx \\
&= x[10]^{-0.7(1-x)^2}(-0.7)(2)(1-x)[\ln(10)](-dx) \\
\frac{da_w}{dx} &= [10]^{-0.7(1-x)^2}[(0.7)(2)(1-x)(x)[\ln 10] + 1]
\end{aligned}$$

Substituting x = 0.9:

$$\begin{aligned}
\left[\frac{da_w}{dx}\right] &= [(0.7)(2)(1-0.9)(0.9)(2.303) + 1][10]^{-0.7(1-0.9)^2} \\
&= 1.3226(10)^{-0.007} = 1.301
\end{aligned}$$

Substituting x = 0.7:

$$\begin{aligned}
\left[\frac{da_w}{dx}\right] &= [(0.7)(2)(1-0.7)(0.7)(2.303) + 1][10]^{-0.7(1-0.7)^2} \\
&= 1.6769(10)^{-0.063} = 1.450
\end{aligned}$$

a_w will be changing faster as x is incremented at x = 0.7 compared to x = 0.9.

Example 1.26. Differentiate:

$$y = \frac{3x+2}{x+3}$$

Using the formula for the derivative of a quotient:

$$dy = \frac{(x+3)d(3x+2) - (3x+2)d(x+3)}{(x+3)^2}$$
$$= \frac{(x+3)(3dx) - (3x+2)dx}{(x+3)^2}$$
$$= \frac{(3x+9-3x-2)dx}{(x-3)^2}$$
$$\frac{dy}{dx} = \frac{7}{(x+3)^2}$$

Example 1.27. The growth of microorganisms expressed as cell mass is represented by the following:

$$\log\left(\frac{C}{C_0}\right) = kt$$

Determine the rate of increase of cell mass at t = 10 hours if it took 1.5 hours for the cell mass to double and the initial cell mass at time zero (C_0) is 0.10 g/L.

Solution:

The value of k is determined from the time required for cell mass to double. $k = (\log 2)/1.5 = 0.200\ h^{-1}$. The expression to be differentiated to determine the rate is $\log(C/0.10) = 0.200t$. Differentiating using the formula for derivative of a logarithmic function:

$$d \log(C/0.10) = 0.200\ dt$$

$$\frac{dC/0.1}{(\ln 10)(C/0.1)} = 0.200\ dt; \quad \frac{dC}{dt} = 0.200C \ln(10) = 0.4605\,C$$

C from the original expression is substituted to obtain a rate expression dependent only on t. $C = C_0(10)^{0.200t}$

$$\frac{dC}{dt} = 0.4605\ C_0\ (10)^{0.200t}$$

At t = 10,

$$\frac{dC}{dt} = 0.4605(0.1)(10)^{2.00} = 4.605 g/L \cdot h$$

1.13.3 Maximum and Minimum Values of Functions

One of the most useful attributes of differential calculus is its use in determining the maximum and minimum values of functions. It has been shown in a previous section that determining a root of a polynomial expression is facilitated by determining where the maximum and minimum points are located. Determination of maximum and minimum values of a function can be applied in optimizing processes to identify conditions where cost is minimum, profit is maximized, or a product quality attribute is maximized.

When a function has a maximum or minimum point, the slope changes signs upon crossing the crest or valley in the curve. Thus at the maximum or minimum point, the slope is zero. After a value of the independent variable is determined at a point where the slope of the curve is zero, that point is identified as a maximum or minimum by either of two methods. (a) Determining the second derivative: As the curve approaches a maximum, the slope is positive and decreases with increasing values of the independent variable, therefore the second derivative is negative. As the curve approaches a minimum, the function has a negative slope that decreases in value, therefore the second derivative is positive. (b) For functions that have a complex second derivative, substitution of the root of the derivative equation into the original function will give the maximum and minimum value of the function. If the derivative equation has only one root, it will be possible to identify this root as the maximum or minimum point by substituting any other value of the independent variable into the original function.

Example 1.28. Plot the curve: $y = 2x^3/3 + x^2 - 6x$ and determine its maximum and minimum value.

Differentiating:

$$\frac{dy}{dx} = 2x^2 + x - 6$$

At the maximum or minimum, $dy/dx = 0$ and $2x^2 + x - 6 = 0$. The roots of the derivative are

$$x = \frac{-1 \pm \sqrt{1 - 4(2)(-6)}}{2(2)}; \quad x = -2; \quad x = 1.5$$

To determine which of these points is a maximum, take the second derivative.

$$\frac{d^2y}{dx^2} = 4x + 1$$

At $x = -2$, $d^2y/dx^2 = -7$. The point is a maximum. Substituting $x = -2$ in the expression for y:

$$y = \frac{2(-2)^3}{3} + \frac{(-2)^2}{2} - 6(-2) = 8.667$$

At $x = 1.5$, $d^2y/dx^2 = 7$. The point is a minimum. Substitute $x = 1.5$ in the expression for y:

$$y = \frac{2(1.5)^3}{3} + \frac{(1.5)^2}{2} - 6(1.5) = -5.625$$

Even without taking the second derivative, values of y show which of the roots of the derivative equation represents the maximum and minimum points.

Example 1.29. Derive an expression for the constants a and b in the equation $y = ax + b$, which is the best-fitting line to a set of experimental data points (x_i, y_i) by minimizing the sum of squares of the error $(y - y_i)$.

$$E = \Sigma(ax_i + b - y_i)^2$$

where $i = 1$ to n. To evaluate a and b, two independent equations must be formulated. E will be maximized with respect to b at constant a, and with respect to a at constant b. x and y are considered constants during the differentiation process with respect to either a or b. The two equations are

$$\frac{dE}{da} = 2\Sigma(ax_i + b - y_i)x_i; \quad \frac{dE}{db} = 2\Sigma(ax_i + b - y_i)$$

The second derivative of these two expressions will be $2\Sigma x_i^2$ and 2, respectively, both of which are positive quantities for all values of a or b; therefore, the root of the derivative equation will represent a point where E is minimum. The two derivative equations are then solved simultaneously.

$$2\Sigma x_i(ax_i + b - y_i) = 0; \qquad 2\Sigma(ax_i + b - y_i) = 0$$

$$b = \frac{\sum y_i - a\sum x_i}{n}; \qquad b = \frac{\sum x_i y_i - a\sum {x_i}^2}{\sum x_i}$$

$$a\Sigma x_i^2 + b\Sigma x_i - \Sigma y_i x_i = 0; \quad a\,\Sigma x_i + nb - \Sigma y_i = 0$$

Equating the two expressions for b and solving for a:

$$a = \frac{\sum x_i y_i - \sum x_i \sum y_i/n}{\sum {x_i}^2 - \left(\sum x_i\right)^2/n}$$

Substituting the expression for a in the expression for b and solving for b:

$$\frac{\Sigma x_i y_i - \Sigma x_i y_i/n}{\Sigma {x_i}^2 - \left(\Sigma x_i\right)^2/n}\Sigma x_i + nb - \Sigma y_i = 0$$

Solving for b:

$$b = \frac{1}{n}\left[\frac{\Sigma y_i \Sigma {x_i}^2 - \Sigma x_i \Sigma x_i y_i}{\Sigma {x_i}^2 - \left(\Sigma x_i\right)^2/n}\right]$$

Example 1.30. Calculate the dimensions of a can that will hold 100 mL of material such that the amount of metal used in its manufacture is a minimum.

Let r = radius and h = height. Two independent equations are needed. One equation must involve the surface area that must be minimized. The other equation must involve the volume because the 100 mL volume requirement must be met. $V = 100 = \pi\, r^2 h$. $h = 100/(\pi\, r^2)$.$A = 2\pi rh + 2\pi r^2$. Substituting h:

$$A = \frac{2\pi(100)}{\pi r^2} + 2\pi r^2 = \frac{200}{r} + 2\pi r^2$$

$$\frac{dA}{dr} = 4\pi r - \frac{200}{r^2} = 0; \quad 4\pi r^3 = 200$$

$$r = \left[\frac{50}{\pi}\right]^{0.333} = 2.51 \text{ cm} \qquad h = \frac{100}{\pi(2.51)^2} = 5.06 \text{ cm}$$

The second derivative, $d^2A/dr^2 = 4\pi + 400\pi/r^3$, will be positive for all positive values of r, therefore the root of the derivative function represents a minimum point. At $r = 2.51$ cm, $A = 2\pi(2.51)^2 + 200/2.51 = 119.3$ cm^2. At $r = 2.4$ cm, $A = 2\pi(2.4)^2 + 200/2.4 = 119.5$ cm^2. The value of A at $r = 2.51$ cm is less than at $r = 2.4$ cm, therefore $r = 2.51$ is a minimum point.

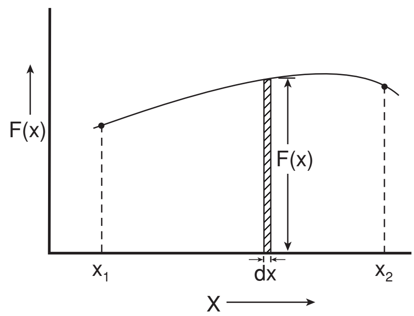


Figure 1.16 Graphical representation of an integral.

1.14 INTEGRAL CALCULUS

Integration is the inverse of differentiation. If dF(x) is the differential term, the integral of dF(x) is F(x). Integrals are differential terms preceded by the integral sign $\int$. The terms inside the integral sign consists of a function F(x) and a differential term dx. Graphically, an integral is represented in Fig. 1.16. The function F(x) traces a curve and the differential term dx is represented by a small area increment with height F(x) and thickness dx. When the area increments are evaluated consecutively, the sum represents the value of the integral. Limits are needed to place a definite value to the integral. The limits must correspond to the value of the variable in the differential term and is the abscissa of the curve used to plot the function within the integral sign. Graphically, the limits define which region of the curve is covered by the area summation. Figure 1.16 represents the graphical equivalent of the following integral

$$\int_{x_1}^{x_2} F(x)dx$$

When evaluating a definite integral, the limits are substituted into the integrand, and the value at the lower limit is subtracted from the value at the upper limit.

When the limits are not specified, the integral is an indefinite integral and the integrand will need a constant of integration $\int F(x) = F(x) + CI$. The value of C is determined using boundary or initial conditions that satisfy the function $F(x) + C$.

1.14.1 Integration Formulas

Only simple and most common integrals are presented here. The reader is encouraged to read a calculus textbook for techniques that are used for more complex functions.

Integral of a sum:

$$\int (du + dv + dw) = \int du + \int dv + \int dw$$

Integral of a power function:

$$\int F(x)^n dF(x) = \frac{F(x)^{n+1}}{n+1} + C$$

Integral of a quotient yielding a logarithmic function:

$$\int \frac{dF(x)}{F(x)} = \ln F(x) + C$$

Integral of an exponential function:

$$\int e^{F(x)} dF(x) = e^{F(x)} + C$$

$$\int 10^{F(x)} dF(x) = \frac{10^{F(x)}}{\ln 10} + C$$

1.14.2 Integration Techniques

1.14.2.1 Constants

Constants may be taken in or out of the integral sign. If only a constant is needed to meet the differential form needed in the above integration formulas, the integral expression may be multiplied and divided by the same constant. The multiplicand is placed within the integral to meet the required differential form, and the divisor is placed outside the integral.

$$\int F(x) dG(x) = F(x)G(x) - \int G(x) dF(x)$$

1.14.2.2 Integration by Parts

$$\int \frac{F(x)dx}{G(x)H(x)} = \int \frac{Adx}{G(x)} + \int \frac{Bdx}{H(x)} + C$$

1.14.2.3 Partial Fractions

A and B are constants obtained by clearing fractions in the above equation and solving for A and B, which would satisfy the equality.

1.14.2.4 Substitution

A variable is used to substitute for a function. The substitution must result in a simpler expression that is integrable using standard integration formulas or integration by parts.

Example 1.31. $\int (x^2 + 3)^2\, dx$.

This does not fit the power function formula because the differential term dx is not $d(x^2 + 3)$. The function can be expanded and integrated as a sum.

$$\int (x^2 + 3)^2 dx = \int (x^4 + 6x^2 + 9)\, dx = \frac{x^5}{5} + \frac{6x^3}{3} + 9x + C$$

Example 1.32.

$$\int_{0.1}^{0.3} (2x^2 + 2)^4 \, x \, dx$$

This function may be integrated using the formula for a power function $d(2x^2 + 2) = 4x\, dx$. The function will be the same as in the power function formula by multiplying by 4. The whole integral is then divided by 4 to retain the same value as the original expression.

$$\int_{0.1}^{0.3} (2x^2 + 2)^4 \, x \, dx = \frac{1}{4} \int_{0.1}^{0.3} (2x^2 + 2)^4 4x \, dx = \frac{1}{4} \frac{(2X^2 + 2)^5}{5} \Big|_{0.1}^{0.3} = \frac{(2.18)^5 - (2.02)^5}{20} = 0.78018$$

Example 1.33. The inactivation of microorganisms under conditions when temperature is changing is given by:

$$\frac{N_0}{N} = \int_0^t \frac{dt}{D_T}$$

N_0 is the initial number of microorganisms, and D_T is the decimal reduction time of the organism. D_T is given by:

$$D_T = D_0[10]^{(250-T)/z}$$

If $D_0 = 1.2$ minutes, $z = 18°F$, $N_0 = 10{,}000$, and $T = 70 + 1.1t$, where T is in °F and t is time in minutes, calculate N at $t = 250$ min. The integral to be evaluated is

$$\frac{10{,}000}{N} = \int_0^{250} \frac{dt}{1.2[10]^{(250-70-1.1t)/18}} = \int_0^{250} \frac{dt}{1.2[10]^{(180-1.1t)/18}}$$

$$= 0.833(10)^{-10} \int_0^{250} (10)^{0.06111t}$$

$$= \frac{1}{1.2(10)^{10}} \int_0^{250} \frac{dt}{(10)^{-0.06111t}}$$

$$= 0.833(10)^{-10} \left[\frac{(10)^{0.06111t}}{0.06111 \ln(10)} \right] \Big|_0^{250}$$

$$= \frac{0.833(10)^{-10}}{0.06111 \ln(10)} [10^{15.275} - 1]$$

The 1 in brackets is much smaller than $10^{15.275}$; therefore, it may be neglected. Therefore:

$$\frac{10{,}000}{N} = 5.9209(10)^{-10}(10)^{15.275}$$

$$= 5.9209(10)^{15.275-10} = 5.9209(10)^{5.275}$$

Taking logarithm of both sides:

$$\log\left(\frac{10{,}000}{N}\right) = 5.275 + \log 5.9209 = 6.047$$

$N = (10)^{4-6.047} = 0.0089$

Example 1.34.

$$\int \frac{xdx}{(2x^2+1)}$$

This function will yield a logarithmic function because the derivative of the denominator is 4x dx. The numerator of the integral can be made the same by multiplying by 4 and dividing the whole integral by 4.

$$\int \frac{xdx}{(2x^2+1)} = \frac{1}{4}\int \frac{4xdx}{(2x^2+1)} = \frac{1}{4}\ln(2x^2+1) + C$$

Example 1.35. Solve for the area under a parabola $y = 4x^2$ bounded by $x = 1$ and $x = 3$ as given by the following integral:

$$A = \int_1^3 4x^2 dx = \frac{4x^3}{3}\bigg|_1^3 = \frac{1}{3}[4(27) - 4] = 34.6667$$

1.15 GRAPHICAL INTEGRATION

Graphical integration is used when functions are so complex they cannot be integrated analytically. They are also used when numerical data are available, such as experimental results, and it is not possible to express the data in the form of an equation that can be integrated analytically. Graphical integration is a numerical technique used for evaluation of differential equations by the finite difference method. Three techniques for graphical integration will be shown. Each of these will be used to evaluate the area under a parabola, solved analytically in the preceding example.

1.15.1 Rectangular Rule

The procedure is illustrated in Fig. 1.17A. The domain under consideration is divided into a sequence of bars. The thickness of the bars represent an increment of x. The height of the bars are set such that the shaded area within the curve that is outside the bar equals the area inside the bar that lies outside the curve. The increments may be unequal, but in Fig. 1.17A equal increments of 0.5 units are used.

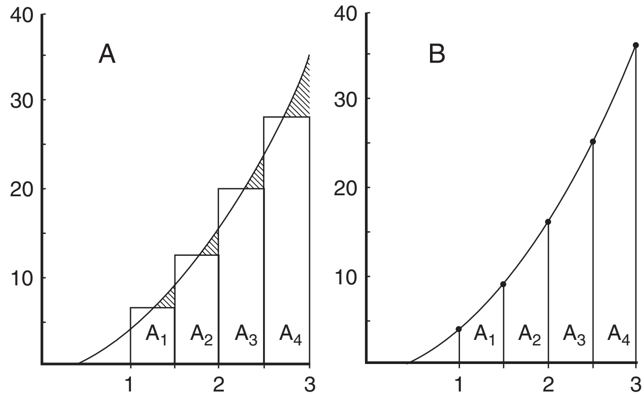


Figure 1.17 Graphical integration by the rectangular (A) and trapezoidal (B) techniques.

The height of the bars are 6.5, 12.5, 20, and 28 for A_1, A_2, A_3, and A_4, respectively. The sum of the area increments is $0.5(6.5 + 12.5 + 20 + 28) = 33.5$

1.15.2 Trapezoidal Rule

The procedure is illustrated in Fig. 1.17B. The domain under consideration is subdivided into a series of trapezoids. The area of the trapezoid is the width multiplied by the arithmetic mean of the height. For the function $y = 4x^2$, the values (height) are 4, 9, 16, 25, and 36, respectively, for x = 1, 1.5, 2, 2.5, and 3. The trapezoids A_1, A_2, A_3, and A_4 will have areas of $0.5(4 + 9)(0.5)$, $0.5(9 + 16)(0.5)$, $0.5(16 + 25)(0.5)$, and $0.5(25 + 36)(0.5)$. The sum is $3.25 + 6.25 + 10.25 + 15.25 = 35$.

1.15.3 Simpson's Rule

This procedure assumes a parabolic curve between area increments. The curve is divided into an even number of increments, therefore, including the value of the function at the lower and upper limits, there will be i values of the height of the function and $(i - 1)$ area increments. The number of increments $(i - 1)$ must be an even integer. Thickness of area increments must be uniform, therefore, for the limits $x = a$ to $x = b$, $\delta x = (b - a)/(i - 1)$. Simpson's rule is as follows:

$$A = \frac{\delta x}{3}[F(a) + 4F(1) + 2F(2) + 4F(3) + 2F(4) \\ + \text{---}\ 2F(i-2) + 4F(i-1) + F(b)]$$

Note the repeating 4, 2, 4, 2, 4 multiplier of the value of the function as succeeding increments are considered. If the index is i = 0 at x = a, the lower limit, all values of the function when the index is even are multiplied by 2 and the multiplier is 4 when the index is odd. For the example of the parabola $y = 4x^2$ from $x = 1$ to $x = 3$, setting the number of increments at 4 gives 5 values of y that must be successively evaluated for the area increment. The thickness of the area increments

$\delta x = (3 - 1)/(4) = 0.5$. Values of F(x) at 1, 1.5, 2, 2.5, and 3 have been determined in the preceding examples. Substituting in the formula for Simpson's rule:

$$A = \frac{0.5}{3}[4 + 4(9) + 2(16) + 4(25) + 36] = 34.6667$$

The accuracy of graphical integration using Simpson's rule is better than the trapezoidal rule. Both the trapezoidal rule and Simpson's rule can be programmed easily in Visual BASIC. The following program in Visual BASIC illustrates how the area of a curve drawn to fit numerical data is determined using Simpson's rule. The area under the parabola $y = 4x^2$ is being analyzed. Smaller thickness of the area increment is used than in the previous example. Ten area increments are chosen, therefore 11 values of the function will be needed to include x = 1 and x = 3, the upper limit.

These values are entered into a Inputbox as variable y with dimension statements.

```
Sub test3()
Dim y (1 to 11) as double
For i = 1 To 11
y(i) = Val(InputBox("Input Data for'' & "Y('' & i & ")''))
next i
i = 11
dx = 0.2
For n = 2 To i Step 2
sa = sa + y(n)
Next n
For n = 3 To i - 1 Step 2
sb = sb + y(n)
Next n
MsgBox "A = '' & (dx / 3)* (4* sa + 2* sb + y(1) + y(11))
End Sub
```

The program, when run, will display A = 34.66667 on the screen.

1.16 DIFFERENTIAL EQUATIONS

Differential equations are used to determine the functionality of variables from information on rate of change. The simplest differential equations are those where the variables are separable. These equations take the form:

$$\frac{dy}{dx} = F(x); \quad dy = F(x)\,dx$$

The solution to the differential equation then involves integration of both sides of the equation. Constants of integration are determined using initial or boundary conditions.

Example 1.36. If the rate of dehydration is constant at 2 kg water/h from a material that weighs 20 kg and contains 80% moisture at time = 0, derive an expression for moisture content as a function of time.

Let W = weight at any time, t = time, and x = moisture content expressed as a mass fraction of water. From the rate data, the differential equation is

$$\frac{dW}{dt} = -2$$

The negative sign arises because the rate is expressed as a weight loss, therefore W will be decreasing with time. Separating variables: $dW = -2dt$. Integrating: $W = -2t + C$. The constant of integration is determined by substituting $W = 20$ at $t = 0$ and the expression for W becomes $W = 20 - 2t$. The moisture content x is determined from W as follows:

$$W = \frac{\text{weight dry solids}}{\text{mass fraction dry solids}} = \frac{20(1 - 0.8)}{1 - x}$$

Substituting W and simplifying:

$$\frac{1}{1 - x} = 5 - 0.5t$$

Example 1.37. The venting of air from a retort by steam displacement is analogous to dilution where the air is continuously diluted with steam and the diluted mixture is continuously vented. Let C = concentration of air at any time, t = time, V = the volume of the retort, and R = the rate of addition of steam. The differential equation for C with respect to time is:

$$V\frac{-dC}{dt} = RC; \ \frac{dC}{C} = \frac{-R}{V}\,dt$$

The integration constant will be evaluated using, as an initial condition, $C = Co$ at $t = 0$. Integrating: $\ln C = (-R/V)t + \ln C_0$.

1.17 FINITE DIFFERENCE APPROXIMATION OF DIFFERENTIAL EQUATIONS

Differential equations may be approximated by finite differences in the same manner as integrals are solved by numerical methods using graphical integration. Finite increments are substituted for the differential terms and the equation is solved within the specified boundaries. Finite difference approximations can be easily done using BASIC.

Example 1.38. A stirred tank having a volume V, in liters, contains a number of cells of microorganisms, N. The tank is continuously fed with cell-free media at the rate of R (L/h) while the volume is maintained constant by allowing media to overflow at the same rate as the feed. The number of cells in the tank will increase due to reproduction, and some of the cells are washed out in the overflow. (a) Derive an equation for the cell number at any time, as a function of the generation time, g, the feed rate, R, and the volume, V. (b) Calculate N after 5 hours, if $g = 0.568$ h, $N_0 = 10{,}000$, $V = 1.5$ L, and $R = 1.5$ L/h.

Solution:

The number of microorganisms in the most rapid rate of growth will increase with time of growth according to: $N = N_0(2)^{t/g}$ where g is generation time. Washout is N(R). Net accumulation is dN/dt (V). Growth $= (dN/dt)_{gr}$ A balance of cell numbers will give: Cell growth = washout +

accumulation.

$$\text{Cell growth} = V\left(\frac{dN}{dt}\right)_{gr} = V\frac{d}{dt}(N_0)(2)^{t/g} = N_0(2)^{t/g}(\ln 2)V = VN\frac{\ln 2}{g}$$

The differential equation is

$$V\,N\frac{\ln 2}{g} = NR + V\frac{dN}{dt}$$

Rearranging and separating variables:

$$\frac{dN}{N} = \left(\frac{\ln 2}{g} - \frac{R}{V}\right)dt$$

Integrating and using as an initial condition $N = N_0$ at $t = 0$:

$$\ln\frac{N}{N_0} = \left(\frac{\ln 2}{g} - \frac{R}{V}\right)t$$

To solve the problem by finite difference techniques, values of V, R, and N_0 and g must be defined. If $g = 0.568$ h, $N_0 = 10{,}000$, $R = 1.5$ L/h, and $V = 1.5$ L, the number of organisms in the tank at $t = 5$ h is as follows: From the analytical solution:

$$\ln N = \ln 10{,}000 + \left[\frac{\ln 2}{0.568} - \frac{1.5}{1.5}\right](5)$$

$$= 9.21 + 1.101 = 10.311$$

$$N = (e)^{10.311} = 30,060$$

The differential equation can be solved using a finite difference technique utilizing Visual BASIC. The program in Visual BASIC for the differential equation is

```
Sub diff()
t = 0
no = 10000
r = 1.5
v = 1.5
g = 0.568
dt = 0.1
n = no
Do
dn = n * (Log(2) / g - (r / v)) * dt
n = n + dn
t = t + dt
Loop While t < 5
MsgBox "time='' & (t - dt) & " n = '' & n
End Sub
```

When the program is run, “Time = 5 N = 30,054.757” will be displayed on the screen.

PROBLEMS

1.1. Determine the maximum and minimum value of the following function and prove that the points are maximum or minimum.

$$C = \frac{315 + 52.5T}{(0.21T - 0.76)^{0.5} - 1.61}$$

1.2. A warehouse having a volume of 10,000 ft^3 and a floor area of 1000 ft^2 is to be built. The cost of constructing the floor is \$6.00/ft^2, the cost of the roof is \$10.00/ft^2, and the cost of the walls is \$20.00/ft^2. If W is the width, L the length, and H the height of the building, what should the dimensions be such that the cost is minimal?

1.3. Calculate the maximum or minimum value of the following expression. Show that the calculated value is maximum or minimum.

$$q = \frac{240R}{-0.02 + 20\ln(0.5/R) + 0.02R}$$

1.4. Calculate the maximum (or minimum value) of y.

$$y = 2X^2 + 0.5R + X + 3$$
$$X = 0.5R$$

1.5. Calculate the maximum velocity of a fluid flowing inside a pipe expressed in terms of the average velocity.
The point velocity (velocity at any point r measured from the center) is

$$V = \left[\frac{\Delta p}{2\ LK}\right]^{1/n} \left[1 - \left[\frac{r}{R}\right]^{(n+1)/n}\right] \left[\frac{n}{n+1}\right] [R]^{(n+1)/n}$$

The average velocity is

$$\overline{V} = \left[\frac{\Delta P}{2\ LK}\right]^{1/n} \left[\frac{n}{3n+1}\right] [R]^{(n+1)/n}$$

1.6. The rate of evaporation of component A divided by the rate of evaporation of component B in a mixture containing A moles of A and B moles of B is directly proportional to A/B. If a mixture originally contained 5 moles of A and 3 moles of B and the rate of evaporation of A is 5 moles/h and of B is 2.6 moles/h, derive an equation for the concentration of A relative to that of B.

1.7. The rate of production of ethanol in a fermentor is directly proportional to the number of cells of yeast present. At a cell mass of 14 g yeast/liter, ethanol production rate is 18 g ethanol/(L $\cong$ h). If a batch fermentor is inoculated with 0.1 g of yeast/L, and the generation time of the yeast is 1.5 hours, what will be the ethanol production after 10 hours of fermentation. Assume no alcohol-induced inhibition of yeast growth and that yeast doubles in cell mass with each generation time.

1.8. The work required to compress a gas is given by the following integral:

$$W = \int_{V_1}^{V_2} P dV$$

Van der Waals equation of state for a gas is is follows:

$$P = \frac{nRT}{V - nb} - \frac{n^2 a}{V^2}$$

$R = 82.06$ ($cm^3 \cong$ atm)/(g mole $\cong$ K), $b = 36.6$ cm^3/g mole, and $a = 1.33 \times 10^6$ (atm $\cong$ cm^6)/(g mole)2, when P is in atm, T in Kelvin, and V in cm^3. Calculate the work done when the pressure of the gas is increased from 1 to 10 atm. There was originally 1 liter of gas at 293 K.

1.9. Write a computer program in BASIC which can be used to calculate a value for the water activity of a solution containing two sugars having mass fractions (percentage composition by weight expressed as a decimal) x_1 and x_2 . x_1 is sucrose (molecular weight 342; $k = 2.7$); x_2 is glucose (molecular weight 180, $k = 0.5$). The water activity of the mixture is

$$a_w = (a_{w1})^0 (a_{w2})^0$$

where $(a_{w1})^0$ is water activity of a solution containing all the water in the mixture and component 1; and $(a_{w2})^0$ is water activity of a solution containing all the water in the mixture and component 2.

$$\log_{10}\left[\frac{(a_{wi})^0}{f_i}\right] = -k_i(1 - f_i)^2$$

where f_i is mole fraction of component i in a solution containing only component i and all the water present in the mixture.

$$f_i = 1 - \left[\frac{x_i/M_i}{(x_i/M_i) + (1 - x_1 - x_2)/18}\right]$$

1.10. Determine the slope of the following functions:

$$f(x) = 2x^4 - 3x^2 + 7 = 0 \quad \text{at } x = 2$$
$$xy = (0.5x + 3)(x + 2) \quad \text{at } x = 1$$

1.11. Determine the maximum and minimum value of the functions in Problem 10 above.

1.12. Determine the slope of the following function at the indicated point.

$$x = (0.5xy + 3)(3 + x^2) \qquad \text{at } x = 1$$

1.13. Construct a spreadsheet that can be used to determine the boiling temperature of a liquid in an evaporator as it is being concentrated. The boiling point of a liquid is the temperature at which the vapor pressure equals the atmospheric pressure. A solution will exhibit a boiling point rise because the solute will lower the water activity resulting in a higher temperature to be reached before boiling occurs. The vapor pressure of water (P^0) as a function of temperature is expressed by the following equation:

$$\ln(P^0) = \left(-\frac{H}{R}\right)\left(\frac{1}{T}\right) + C$$

where P^0 is the vapor pressure in kilopascals, H/R is the ratio of the latent heat of vaporization and the gas constant, C is a constant, and T is the absolute temperature in degrees Kelvin. The value for H/R is 4950 and C is 17.86.

Atmospheric pressure is 101 kilopascals. The vapor pressure of a solution is $P = a_w P^0$. The water activity (a_w) is given by:

$$\log_{10}\left(\frac{a_w}{f_1}\right) = -k(1 - f_1)^2$$

f_1 is the mole fraction of water and is calculated by:

$$f_1 = \frac{(1 - x_1)/18}{(1 - x_1)/18 + x_1/M_1}$$

x_1 is the mass fraction of solute. Assume the solute is only sucrose with a molecular weight (M_1) of 342 and a k value of 2.7. Have the program display the value of the boiling point when the sucrose concentration is 20% and at increasing concentrations in 5% intervals to a final concentration of 60%.

1.14. Calculate a value of x that would give the minimum value for S in the following expression:

$$S = 50(9.522 \times 10^{-6}) - \frac{50}{(50X + 1)}(9.522 \times 10^{-6}) - \frac{60(0.22)X}{30(24)}$$

Show that the function is a minimum or maximum.

1.15. In the dehydration of diced potatoes, the following weights were recorded at various times in the process when dehydration rate was the slowest.

$t = 6$ hours from start of drying: weight $= 2350$ g
$t = 8$ hours from start of drying: weight is 2275 g; moisture content $= 15.6\%$.

In this range of moisture content, the drying rate is proportional to the moisture content, expressed in mathematical form as follows:

$$-\frac{dW}{dt} = kW$$

W is the moisture content in g water/g dry matter, and k is a constant.

(a) Derive an equation for the moisture content, W, as a function of time, t, which satisfies the experimental conditions given above.
(b) How long would it take for a product to be dehydrated from 22.5% to 12.5% moisture?

$$\frac{N_0}{N} = \frac{R^2\overline{V}}{2}\left[\frac{1}{\int_0^R rV_r[10]^{-L/(V_rD)}dr}\right]$$

1.16. Write a computer program in BASIC that will solve the following integral:
where

$$V_r = \overline{V}\left[\frac{3n+1}{n+1}\right]\left[1 - \frac{r}{R}^{(n+1)/n}\right]$$

Given: $\overline{V} = 2$, $R = 0.02$, $n = 0.6$, $L = 10$, $D = 1$. Use the trapezoidal rule in evaluating the integral and use increments in r of 0.0001.

1.17. Linearize the following equations. In each case, indicate which function should be plotted as the independent and dependent variable to obtain a linear plot. What is the slope and intercept of each plot?

(a) $\log(a_w/X_i) = -k(1 - X_i)^2$ where a_w and X_i are variables.

(b) $(1/x) = (a + b)/2y + c/4y$ where x and y are variables and a, b, and c are constants.

(c) $N = N_0(10)^{-(t/D)}$ where N and t are variables and N_0 and D are constants.

1.18. The velocity of an enzyme-catalyzed reaction (V) expressed as a function of the substrate

$$V = \frac{V_{max}(S)}{K_m + S}$$

concentration (S) is given by the following equation:
where V_{max} is the maximum reaction rate and K_m is a constant for the reaction. Linearize the equation and determine the independent and dependent variables to be plotted to obtain V_{max} and K_m from the slope and intercept.

1.19. The temperature (T) of a refrigerant during compression in a refrigeration system increases with pressure (P) as shown in the following equation. P_1 and T_1 are reference temperature and pressure and are considered constants.

$$\frac{T}{T_1} = \left[\frac{P}{P_1}\right]^{(k-1)/k}$$

The following data are available on the temperature and pressure of a refrigerant during compression:

T(ER)	450	510	550	608	640
$P(lb_f/in^2)$	4	6	10	20	30

Linearize the above equation, perform a linear regression, and determine the constant k for this refrigerant. Calculate the value of k by nonlinear curve fitting.

1.20. The heat of respiration of leafy greens as a function of time when the temperature is changing during a cooling operation is as follows:

$$q = \int_0^t 0.009854[e]^{0.073T}\,dt$$

where q is in BTU/(lb), T is in °F, and t is time in hours. The temperature of a box of spinach containing 50 lb, originally at 110°F, will cool down exponentially when placed in a refrigerated room at 35°F according to:

$$T = 35 + (75)\exp(-t/5)$$

where t is the time in hours. Evaluate this integral using a spreadsheet and determine the total heat generated by the spinach as the box cools down from 110°F to 40°F. Use Simpson's rule to determine the value of the integral.

1.21. An immobilized enzyme reactor must have the enzyme regenerated periodically because of the decay in the activity of the enzyme. The enzyme will convert 87% of the substrate to product within the first day of operation, and this conversion changes to $0.87/(t)^{0.82}$ after the first day. If the feed rate is 150 lb of substrate per day, the amount of product formed after t days of operation will be:

$$P = 150(0.87) + \left[\frac{150(0.87)}{(t)^{0.82}}\right](t - 1)$$

At a substrate cost of \$2.50/lb, an operating cost of \$600.00/day, a product cost of \$14.00/lb, and an enzyme replacement cost of \$600, the return from the operation will be

$$S = 14P - 600(t) - 2.5(P) - 600/t$$

Calculate the number of days t that the reactor must be operated before recharging in order that the return, S, will be maximum. Prove that S is maximum at the value of t identified.

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