2.2.1 MATLAB Software

MATLAB is an integrated technical computing environment that combines numeric computation, advanced graphics and visualization, and a high-level programming language. The MATLAB software was originally developed to be a matrix laboratory (MATrix LABoratory). Its capabilities have expanded greatly in recent years and is today a leading tool for engineering computation. Because MATLAB commands are similar to the way we express engineering concepts in mathematics, writing computer programs in MATLAB is much quicker than writing computer code in languages such as FORTRAN or C. Also, MATLAB provides excellent graphics capability that is easy to use. The MATLAB software consists of a basic package of mathematical routines as well as optional **toolboxes** that cover specific engineering application areas such as process control, neural networks, optimization, signal processing and symbolic mathematics. It also has a toolbox that makes available many of the NAG (Numerical Algorithms Group) routines. These routines are some of the best implementations of numerical methods that are currently available. MATLAB now offers a convenient computing environment for the solution of process simulation problems and will be used extensively in this book.

Several excellent books have been written that assist a new user of MATLAB. These include those by Etter (1993), Biran and Breiner (1995), and the Math Works, Inc. (1995). To begin MATLAB, select MATLAB from your program manager menu. You start programming when you see the MATLAB prompt (≫). MATLAB uses two windows: a command window to enter commands and data and to print results, and a graphics window to generate plots. An important command is the abort command (`∧C` or control C). Often a mistake has been made and extraneous output is being displayed or you find yourself in a seemingly endless loop. At this point you want to abort the run. MATLAB commands are usually entered on separate lines. Multiple statements can be entered on the same line if separated by semicolons. A line can be continued to the next line by using ... at the end of the line. Comments can be entered on a line following following a percent sign (`%`). The `help` command is an important resource. When you enter the command `help`, a list of help topics is displayed (See Appendix B, Table B.1). You can then select the topic on which you require information. Specific topics are then displayed. You can then enter `help` on the specific topic to learn details about it.

In addition to executing commands entered through the keyboard, you can also use commands stored as files. These files all end in the extension `.m` and are called M-files because of the file name extension. Long programs are usually created in a text editor and stored as an M-file that can be executed in a MATLAB session. Short programs are usually created and run directly on-line. Since MATLAB is an interpreter language, you must have a correct executable statement before the next statement can be entered.

Appendix B gives reference tables on aspects of MATLAB that will be used in this book.

2.2.2 Linear Algebra Routines Available in MATLAB

Essentially two operations are available in MATLAB for solving linear algebraic equations

$$\boldsymbol{Ax} = \boldsymbol{b} \tag{2.2.30}$$

The first is the use of the inverse operation `inv` (Table B.18)

$$\gg \quad \texttt{x} = \texttt{inv}\ (\texttt{A}) * \texttt{b} \tag{2.2.31}$$

A more efficient method is the use of the \ or / operation which solves the set of equations using ***LU*** factorization and Gaussian elimination (Table B.18).

$$\gg \quad \texttt{x} = \texttt{A} \backslash \texttt{b} \tag{2.2.32}$$

The \ operation is the left division and / is right division. In this case, left division is used since the matrix $\boldsymbol{A}$ is to the left of vector $\boldsymbol{b}$. You can learn about these operations in MATLAB by entering `help slash`. The right division $\boldsymbol{B}/\boldsymbol{A}$ computes $(\boldsymbol{A}^T/\boldsymbol{B}^T)^T$ again using ***LU*** factorization and Guassian eliminination.

The ***LU*** factorization of the $\boldsymbol{A}$ matrix is available using the `lu` function in MATLAB (Table B.18).

$$\gg \quad [\texttt{L}, \texttt{U}, \texttt{P}] = \texttt{lu}\ (\texttt{A}) \tag{2.2.33}$$

where $\boldsymbol{L}$ is the lower triangular matrix with unity down the diagonal, $\boldsymbol{U}$ is an upper triangular matrix, and $\boldsymbol{P}$ a permutation matrix that keeps track of any row shifting. The result of this algorithm is

$$\boldsymbol{PA} = \boldsymbol{LU} \tag{2.2.34}$$

EXAMPLE 2.1 Six-Plate Absorption Column:

It is desired to develop the steady–state tray compositions for a six–plate absorption column. It can be assumed that a linear equilibrium relation holds between liquid (x_m) and vapor (y_m) on each plate:

$$y_m = ax_m + b \tag{2.2.35}$$

The inlet composition to the column x_0 and y_7 are specified along with the liquid (L) and gas (G) phase flow rates (moles/time). The system is shown schematically in Figure 2.1.

To solve the problem, a material balance is written on a representative tray, n, shown in Figure 2.2.

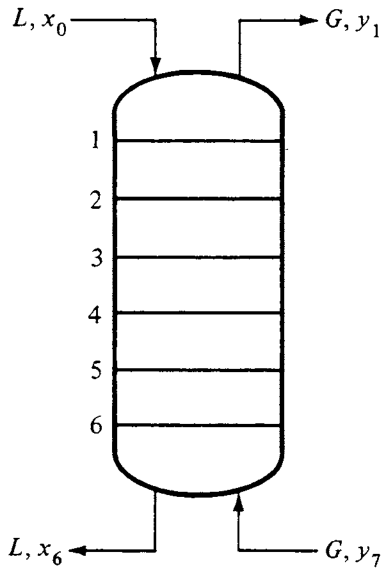

Figure 2.1: Absorption Column.

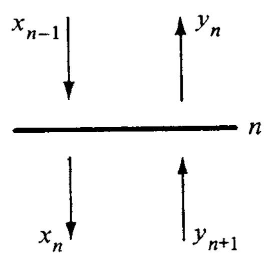

Figure 2.2: Typical Tray.

Applying the macroscopic mass balance yields

$$\begin{gathered}\text{Rate of mass in} = \text{Rate of mass out}\\ Lx_{n-1} + Gy_{n+1} = Lx_n + Gy_n\end{gathered} \tag{2.2.36}$$

Using the linear equilibrium relation in the mass balance gives

$$Lx_{n-1} + G(ax_{n+1} + b) = Lx_n + G(ax_n + b) \tag{2.2.37}$$

or

$$Lx_{n-1} - (L + Ga)x_n + Gax_{n+1} = 0 \tag{2.2.38}$$

The entire set of equations for the six-plate column is

$$\begin{array}{ll} -(L+Ga)x_1 + Gax_2 = -Lx_0 & \text{(where } x_0 \text{ is specified)} \\ Lx_1 - (L+Ga)x_2 + Gax_3 = 0 & \\ Lx_2 - (L+Ga)x_3 + Gax_4 = 0 & \\ Lx_3 - (L+Ga)x_4 + Gax_5 = 0 & \\ Lx_4 - (L+Ga)x_5 + Gax_6 = 0 & \\ Lx_5 - (L+Ga)x_6 = -Ga\frac{y_7-b}{a} & \text{(where } y_7 \text{ is specified)} \end{array} \tag{2.2.39}$$

The simultaneous solution can be expressed in matrix notation as

$$\begin{bmatrix} -(L+Ga) & Ga & & & & \\ L & -(L+Ga) & Ga & & & \\ & L & -(L+Ga) & Ga & & \\ & & L & -(L+Ga) & Ga & \\ & & & L & -(L+Ga) & Ga \\ & & & & L & -(L+Ga) \end{bmatrix}$$

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{bmatrix} = \begin{bmatrix} -Lx_0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -Ga\frac{y_7-b}{a} \end{bmatrix} \tag{2.2.40}$$

The matrix equation is

$$\boldsymbol{Ax} = \boldsymbol{b} \tag{2.2.41}$$

We want to compute the solution vector $\boldsymbol{x}$.

A typical set of parameters for this problem is

$$\begin{array}{ll} a = 0.72 & G = 66.7 \text{ kg mol/min} \\ b = 0 & L = 40.8 \text{ kg mol/min} \end{array}$$

We would like to solve for two cases. The first is when the liquid feed is pure ($x_0 = 0$) and the gas feed is 0.2 kg mol solute/kg mol inert ($y_7 = 0.2$). The second case is $x_0 = 0$ and $y_7 = 0.3$. Figure 2.3 shows a MATLAB file `lin2_1.m` that solves this problem. This file is available from the world wide web under: `http://optimal.colorado.edu/~ramirez/chen4580.html`. This M-file first defines the constants for the problem. It then generates the $\boldsymbol{A}$ matrix and two $\boldsymbol{b}$ vectors each associated with the two cases of interest for $y_7 = .2$ and $y_7 = .3$. Solutions to the problem are obtained both using in `inv` function and the Gaussian elimination procedure using the left division operation \. When you run this M-file, you will obtain the results shown as comment lines at the end of this file. Note that to the accuracy given in the default output the results are equivalent using either approach.

Figure 2.3: MATLAB M-file `lin2_1.m` to solve EXAMPLE 2.1

```
% This is the M-file for solving the set of linear equations
% described in EXAMPLE 2.1.

%
% read in process parameters:
%
a = 0.72;
b = 0;
G = 66.7;
L = 40.8;

%
% read in initial conditions
%
x0 = 0; y7(1) = 0.2; y7(2) = 0.3;

%
% read in matrices A and B:
%
A = zeros(6);
A(1,1) = -(L+G*a);
A(2,1) = L;
A(1,2) = G*a;
A(2,2) = -(L+G*a);
A(3,2) = L;
A(2,3) = G*a;
A(3,3) = -(L+G*a);
A(4,3) = L;
A(3,4) = G*a;
A(4,4) = -(L+G*a);
A(5,4) = L;
A(4,5) = G*a;
A(5,5) = -(L+G*a);
A(6,5) = L;
A(5,6) = G*a;
A(6,6) = -(L+G*a);

B1 = zeros(6,1);
B1(1,1) = -L*x0;
B1(6,1) = -G*a*(y7(1)-b)/a;

B2 = zeros(6,1);
B2(1,1) = -L*x0;
B2(6,1) = -G*a*(y7(2)-b)/a;

%
% solve for the tray compositions:
%

%
% if you want to display the results with long format, use:
```

```
% (see "help format" for more info.)
%
%format long

%
% use matrix inversion:
%
x1 = inv(A)*B1
x2 = inv(A)*B2

%
% for better numerical accuracy, use Gaussian elimination:
%
x1 = A\B1
x2 = A\B2


%
%=========
% results
%=========
%>> linear2_1
%

% results using matrix inversion

%x1 =
%
%    0.0614
%    0.1136
%    0.1579
%    0.1955
%    0.2275
%    0.2547


%x2 =

%    0.0921
%    0.1703
%    0.2368
%    0.2933
%    0.3413
%    0.3820
%
% results using matrix division

%x1 =

%    0.0614
%    0.1136
%    0.1579
%    0.1955
```

```
%     0.2275
%     0.2547

%x2 =

%     0.0921
%     0.1703
%     0.2368
%     0.2933
%     0.3413
%     0.3820
```

EXAMPLE 2.2 Material Balances for Alcohol Distillation:

A company plans to make commercial alcohol by the distillation process shown in Figure 2.4. The process contains two distillation columns, both having reflux ratios of three to one. A feed of 10000 kg/hr is 80 percent (wt) water, 10 percent alcohol, and 10 percent organic material. The distillate from the first column is 60 percent alcohol while that from the second column is 95 percent. The bottom stream from the first column contains 80 percent of the organic material feed while the rest leaves the bottom of the second column. No alcohol is present in either of the bottom streams. Solve for the amount of each component in each stream.

Component material balances are written for the system. The component material balances written around a control volume which includes both still 1 and condenser 1 are

$$W_2 = W_7 + W_6 \quad (7)$$
$$A_2 = A_7 \quad (10)$$
$$R_2 = R_7 + R_6 \quad (11)$$

The reflux specifications are

$$W_5 - 3W_7 = 0 \quad (4)$$
$$A_5 - 3A_7 = 0 \quad (5)$$
$$R_5 - 3R_7 = 0 \quad (6)$$

and the material balances describing the split leaving condenser 1 can be expressed as

$$W_3 - \tfrac{4}{3}W_5 = 0 \quad (1)$$
$$A_3 - \tfrac{4}{3}A_5 = 0 \quad (2)$$
$$R_3 - \tfrac{4}{3}R_5 = 0 \quad (3)$$

Material balances written around a control volume which includes still 2, condenser 2, and heat exchanger 1 are

$$W_7 = W_{13} + W_{12} \quad (16)$$
$$A_7 = A_{13} \quad (19)$$
$$R_7 = R_{12} \quad (17)$$

The reflux specifications are

$$W_{11} - 3W_{13} = 0 \quad (14)$$
$$A_{11} - 3A_{13} = 0 \quad (15)$$