IDEAL BINARY DISTILLATION

MODULE 10

After studying this module, the student should be able to

- Develop the dynamic modeling equations for ideal binary distillation
- Solve for the steady-state
- Linearize and find the state space model
- Understand the dynamic behavior of distillation columns
- Use MATLAB for steady-state and dynamic simulation

The major sections of this module are:

M10.1   Background
M10.2   Conceptual Description of Distillation
M10.3   Dynamic Material Balances
M10.4   Solving the Steady-State Equations
M10.5   Solving the Nonlinear Dynamic Equations
M10.6   State-Space Linear Distillation Models
M10.7   Multiplicity Behavior

M10.1   BACKGROUND

Distillation is a common separation technique for liquid streams containing two or more components and is one of the more important unit operations in chemical manufacturing processes. Design and control of distillation is important in order to produce product streams of required purity, either for sale or for use in other chemical processes.
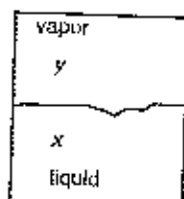
FIGURE M10.1   Closed system with
liquid and vapor in equilibrium.

Distillation is based on the separation of components of a liquid mixture by virtue
of the differences in boiling points of the components. For illustration purposes, we will
base our discussion on the separation of liquid streams containing two components (bi-
nary mixture). We will refer to the pure component that boils at a lower temperature as
the *light* component and the pure component that boils at a higher temperature as the
heavy component. For example, in a mixture of benzene and toluene, benzene is the light
component and toluene is the heavy component.

A saturated liquid mixture of two components at a given concentration is in equilib-
rium with a vapor phase that has a higher concentration of the light component than the
liquid phase. Let x represent the mole fraction of the light component in the liquid phase
and y represent the mole fraction of the light component in the vapor phase. Consider Fig-
ure M10.1 as a conceptual representation of phase (vapor/liquid) equilibrium. The satu-
rated liquid is in equilibrium with a saturated vapor. The concentration of the light com-
ponent will be larger in the vapor phase than the liquid phase.

Figure M10.2 is an example of an equilibrium diagram that represents the relation-
ship between the liquid and vapor phase compositions (mole fraction). For example, if the
liquid composition is 0.5 mole fraction of the light component, we find from Figure
M10.2 that the vapor composition is 0.7.
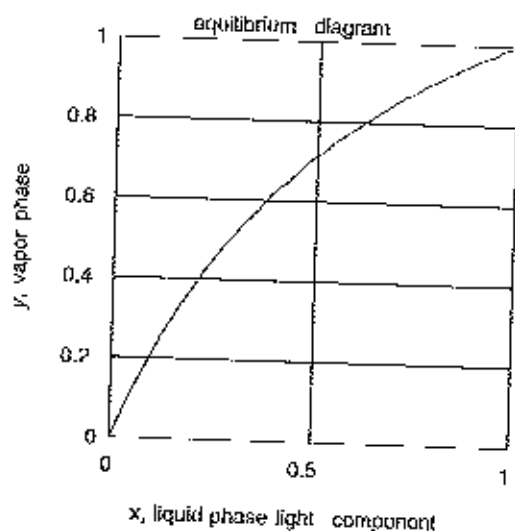

x, liquid phase light   component

FIGURE M10.2   Vapor/liquid
equilibrium diagram.

For ideal mixtures, it is common to model the phase equilibrium relationship based on constant relative volatility

$$y = \frac{\alpha x}{1 + (\alpha - 1)x} \tag{M10.1}$$

where α is known as the relative volatility. Figure M10.2 was generated based on equation (M10.1) with $\alpha = 2.5$.

M10.2 CONCEPTUAL DESCRIPTION OF DISTILLATION

The following is a conceptual description of the operation of a binary (two-component) distillation column. The feed typically enters close to the middle of the column (above the feed stage), as shown in Figure M10.3. Vapor flows from stage to stage up the column, while liquid flows from stage to stage down the column. The vapor from the top tray is condensed to liquid in the overhead condenser and a portion of that liquid is returned as reflux. The rest of that vapor is withdrawn as the overhead product stream; this overhead product stream contains a concentrated amount of the light component. A portion of the liquid at the bottom of the column is withdrawn as a bottoms product (containing a con-
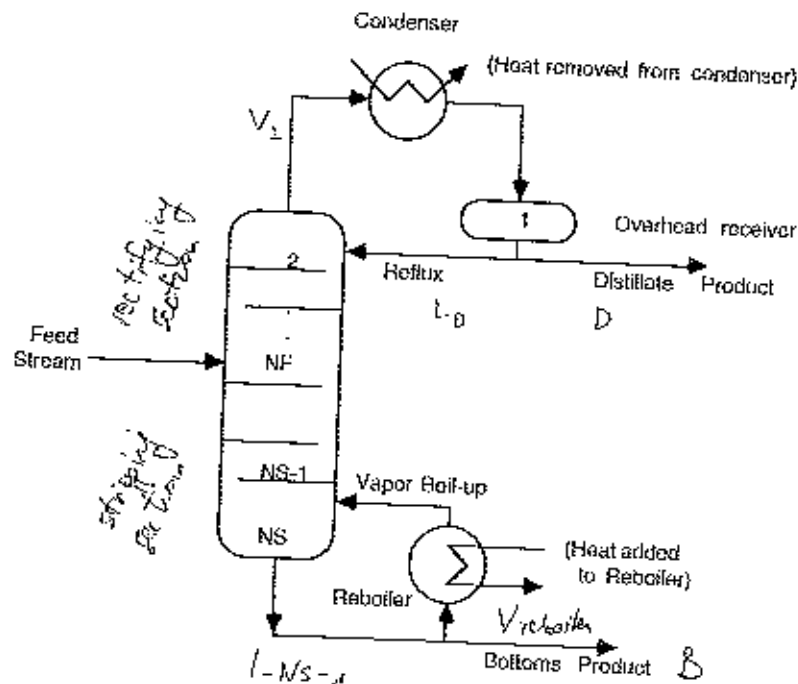

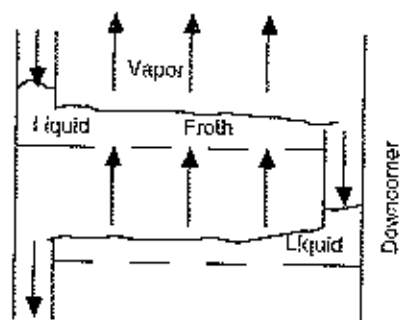FIGURE M10.3   Schematic diagram for a distillation column.

FIGURE M10.4   Schematic diagram for a distillation column tray.

centrated amount of the heavy component), while the rest is vaporized in the reboiler and returned to the column.

The liquid from one tray goes over a weir and cascades down to the next tray through a downcomer. As the liquid moves across a tray, it comes in contact with the vapor from the tray below. The schematic diagram for a sieve tray is shown in Figure M10.4.

Generally, as the vapor from the tray below comes in contact with the liquid, turbulent mixing is promoted. Assuming that the mixing is perfect, allows one to model the stage as a lumped parameter system, as shown in Figure M10.5. Notice that the vapor from stage i is modeled as a single stream with molar flowrate V_i and light component vapor composition (mole fraction) y_i. The liquid leaving stage i through the downcomer is modeled as a single stream with molar flowrate L_i and light component liquid composition (mole fraction) x_i.

The conceptual diagram for the feed stage is shown in Figure M10.6. It differs from Figure M10.5 in that an additional input to the stage is from the feed to the column.
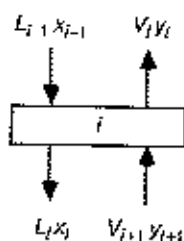

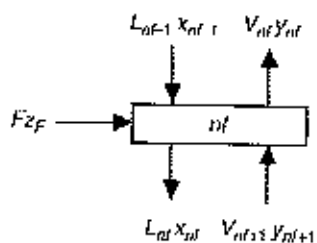**FIGURE M10.5**   Conceptual material balance diagram for a typical stage.

FIGURE M10.6   Conceptual material balance diagram for the feed stage.

M10.3 DYNAMIC MATERIAL BALANCES

M10.3.1 All Stages Except Feed, Condenser, and Reboiler

The component balance for the liquid phase of a typical stage as shown in Figure M10.5 is:

accumulation   liquid from   vapor from   liquid   vapor
              tray above   tray below   leaving leaving

$$\frac{dM_i x_i}{dt} = L_{i-1} x_{i-1} + V_{i+1} y_{i+1} - L_i x_i - V_i y_i \tag{M10.2}$$

where M_i is the liquid molar holdup on stage i.

For this simple binary distillation model, we will make the common assumption of equimolal overflow (King, 1980). For any stage except the feed stage, we assume that the vapor flowrate from one stage is equal to the vapor molar flowrate of the stage below:

$$V_i = V_{i+1} \tag{M10.3}$$

and that the liquid leaving the stage is equal to the liquid flowing from one stage above:

$$L_i = L_{i-1} \tag{M10.4}$$

M10.3.2 Feed Stage

Let q_F represent the *quality* of the feedstream. If the feed is a saturated liquid, then $q_F = 1$, while $q_F = 0$ for a saturated vapor. The vapor molar flowrate leaving the feed stage is (where NF = number of the feed stage)

$$V_{NF} = V_{NF+1} + F(1 - q_F) \tag{M10.5}$$

Similarly, the liquid molar flowrate of the stream leaving the feed stage is:

$$L_{NF} = L_{NF-1} + F q_F \tag{M10.6}$$

M10.3.3 Condenser

A total condenser removes energy from the overhead vapor, resulting in a saturated liquid. Assuming a constant molar holdup in the distillate receiver, the total liquid flowrate from the distillate receiver (reflux + distillate flows) is equal to the flowrate of the vapor from the top tray:

$$L_R + D = V_2 \tag{M10.7}$$

where L_R and D represent the reflux and distillate molar flowrates, respectively.
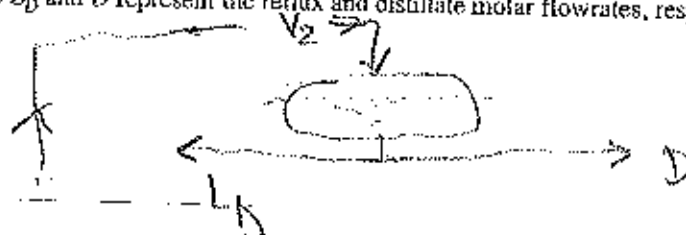
M10.3.4   Reboiler

A total material balance around the reboiler yields:

$$B = L_{NS-1} - V_{reboiler} \qquad (M10.8)$$

where $V_{reboiler}$ is the reboiler molar flowrate and B is the bottoms product molar flowrate.

M10.3.5   Summary of the Modeling Equations

The rectifying section (top section of column, above the feed stage) liquid molar flowrates are:

$$L_R = L_D \qquad (M10.9)$$

The stripping section (bottom section of column, below the feed stage) liquid molar flowrates are

$$L_S = L_R + Fq_F \qquad (M10.10)$$

The stripping section vapor molar flowrates are:

$$V_S = V_{reboiler} \qquad (M10.11)$$

The rectifying section vapor molar flowrates are:

$$V_R = V_S + F(1 - q_F) \qquad (M10.12)$$

In the following we assume a constant liquid phase molar holdup $(dM/dt) = 0$. The overhead receiver component balance is:

$$\frac{dx_1}{dt} = \frac{1}{M_D}[V_R(y_2 - x_1)] \qquad (M10.13)$$

The rectifying section component balance is (from $i = 2$ to $NF-1$):

$$\frac{dx_i}{dt} = \frac{1}{M_T}[L_R x_{i-1} + V_R y_{i+1} - L_R x_i - V_R y_i] \qquad (M10.14)$$

The feed stage balance is:

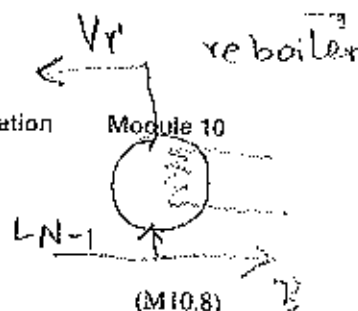$$\frac{dx_{NF}}{dt} = \frac{1}{M_T}[L_R x_{NF-1} + V_S y_{NF+1} + Fz_F - L_S x_{NF} - V_R y_{NF}] \qquad (M10.15)$$

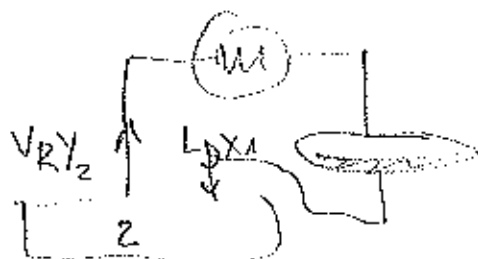The rectifying section component balance is (from $i = NF+1$ to $NS-1$):

$$\frac{dx_i}{dt} = \frac{1}{M_T}[L_S x_{i-1} + V_S y_{i+1} - L_S x_i - V_S y_i] \qquad (M10.16)$$

And the reboiler component balance is:

$$\frac{dx_{NS}}{dt} = \frac{1}{M_B}[L_S x_{NS-1} - Bx_{NS} - V_S y_{NS}] \qquad (M10.17)$$

EQUILIBRIUM RELATIONSHIP

It is assumed that the vapor leaving a stage is in equilibrium with the liquid on the stage. The relationship between the liquid and vapor phase concentrations on a particular stage can be calculated using the constant relative volatility expression:

$$y_i = \frac{\alpha x_i}{1 + (\alpha - 1)x_i} \qquad (M10.18)$$

M10.4 SOLVING THE STEADY-STATE EQUATIONS

To obtain the steady-state concentrations we must solve the system of equations, $f(x) = 0$. From the overhead receiver component balance:

$$f_1 = y_2 - x_1 = 0 \qquad (M10.19)$$

From the rectifying section component balance ($i = 2$ to $NF-1$):

$$f_i = L_R x_{i-1} + V_R y_{i+1} - L_R x_i - V_R y_i = 0 \qquad (M10.20)$$

From the feed stage balance:

$$f_{NF} = L_R x_{NF-1} + V_S y_{NF+1} + F z_F - L_S x_{NF} - V_R y_{NF} = 0 \qquad (M10.21)$$

From the stripping section component balance ($i = NF+1$ to $NS-1$):

$$f_i = L_S x_{i-1} + V_S y_{i+1} - L_S x_i - V_S y_i = 0 \qquad (M10.22)$$

And from the reboiler component balance:

$$f_{NS} = L_S x_{NS-1} - B x_{NS} - V_S y_{NS} = 0 \qquad (M10.23)$$

where $B = L_S - V_S$.

We must realize that (M10.19)–(M10.23) constitute a set of nonlinear algebraic equations, since the relative volatility relationship (M10.18) is nonlinear in the state variable. Equations (M10.19)–(M10.23) are NS equations in NS unknowns. A Newton-based technique will be used to solve the equations.

EXAMPLE M10.1   Steady-State Operation of a 41-Stage Column

Consider a 41-stage column with the overhead condenser as stage 1, the feed tray as stage 21 and the reboiler as stage 41. The following parameters and inputs apply

$$\begin{aligned}
\alpha &= 1.5 \\
F &= 1 \text{ mol/min} \\
z_F &= 0.5 \text{ mole fraction of light component} \\
R &= 2.706 \text{ mol/min} \\
D &= 0.5 \text{ mol/min} \\
q_F &= 1 \text{ (sat'd liquid feed)}
\end{aligned}$$

$- L_D = reflux$

From an overall material balance, the bottoms product flowrate is:

$$B = F - D = 1 - 0.5 \text{ mol/min}$$

the stripping section flowrate is:

$$L_s = R + Fq_F = 2.706 + 1 = 3.706 \text{ mol/min}$$

and a balance around the reboiler yields:

$$V_S = L_S - B = 3.706 - 0.5 = 3.206 \text{ mol/min}$$

The m-file dist_ss.m (shown in the Appendix) is used to solve for the steady-state compositions.

$$x = \text{fsolve('dist\_ss',x0)}$$

The resulting compositions are shown in Figure M10.7. Notice the strong sensitivity to reflux flowrate.
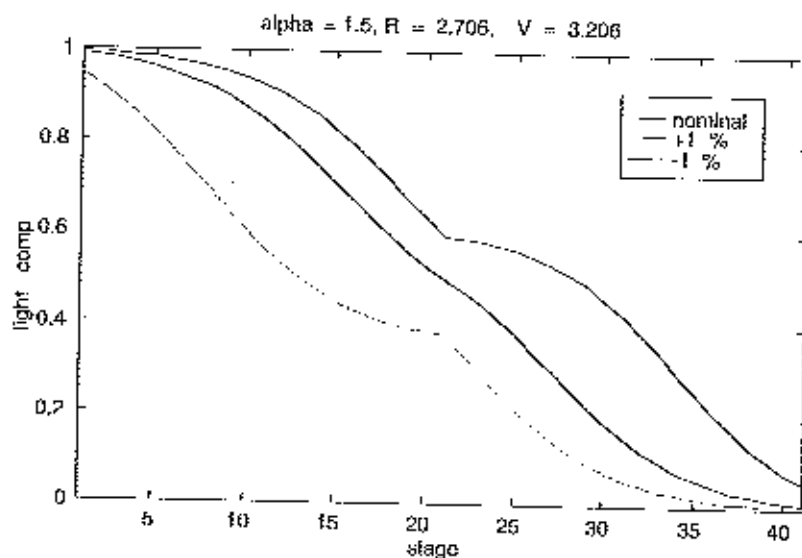
FIGURE M10.7　Liquid phase composition (mol fraction of light component) as a function of stage number. Solid = nominal reflux, dashed = +1% reflux, dotted = −1% reflux.

The overhead composition (stage 1) is 0.99 and the bottoms composition (stage 41) is 0.01 for the nominal reflux rate (2.706 mol/min).

Steady-State Input-Output Relationships

The sensitivity to reflux rate is also shown by the plot in Figure M10.8. The steady-state gain (change in output/change in input) for distillate composition is large when reflux is less than 2.7,

but small when the reflux is greater than 2.71 mol/min. The opposite relationship holds for bot toms composition, where the gain is small when reflux is less than 2.7 mol/min, but large for reflux greater than 2.71 mol/min. This sensitivity has important ramifications for control system design.
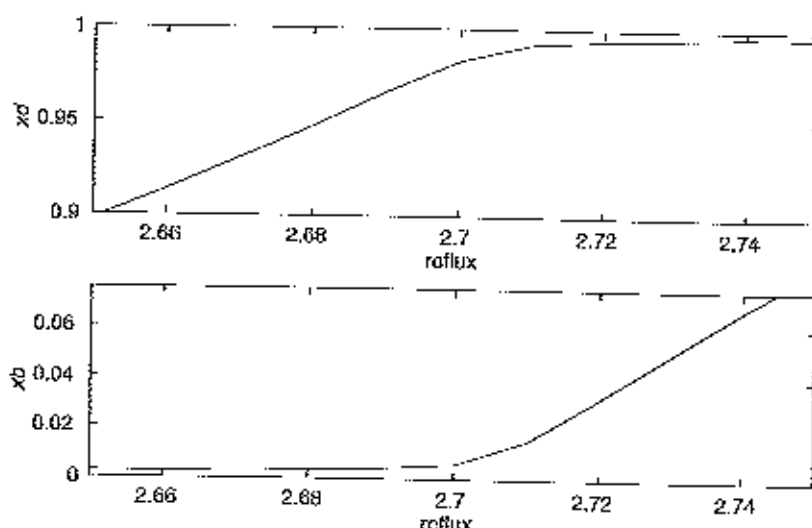
FIGURE M10.8   Steady-state input (reflux) –output (distillate or bottoms composition) relationship.

M10.5   SOLVING THE NONLINEAR DYNAMIC EQUATIONS

Equations (M10.13) (M10.17) are a set of initial value ordinary equations, which can be solved using numerical integration techniques. The next example uses the variable step size MATLAB routine ode45 to perform the integration.

EXAMPLE M10.2   Dynamic Response

Consider now the previous problem, with the initial conditions of the stage compositions equal to the steady-state solution of Example M10.1. The additional parameters needed for the dynamic simulation are the molar holdups on each stage. Here we use the following parameters:

$$
\begin{aligned}
M_1 = M_D &= \text{overhead receiver molar holdup} &= 5 \text{ mol} \\
M_2 &= \text{feed tray molar holdup} &= 0.5 \text{ mol} \\
M_3 = 5 &= \text{bottoms (reboiler) molar holdup} &= 5 \text{ mol}
\end{aligned}
$$

To illustrate the nonlinear behavior we compare the results of ± 1% step changes in the reflux rate at time t = 5 minutes.

```
[t,x]=ode45('dist_dyn',0,400,x0)
```

Note that the current version of ode45 does not allow model parameters to be passed through the argument list, so global parameters are defined in the m-file dist_dyn.m shown in the Appendix.

The following results are shown in Figure M10.9. A positive 1% step change in the reflux rate yields a small increase in the distillate composition; this makes sense because the maximum possible increase in distillate purity is 0.01 (the composition cannot be greater than 1 mole fraction) while it can decrease much more than that. A negative 1% step change in reflux causes a larger change in the distillate purity. The opposite effects are observed for bottoms composition, where a positive reflux change yields a large bottoms composition change. A negative reflux change yields a small bottoms composition change.

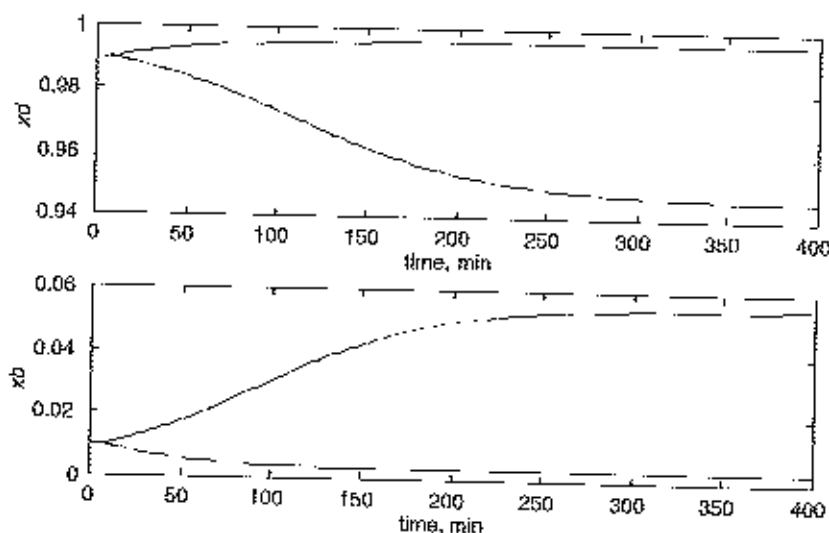**FIGURE M10.9**   Illustration in nonlinear response of distillate and bottoms compositions to step changes in reflux. Solid line = +1%, Dashed line = −1%.

M10.6   STATE-SPACE LINEAR DISTILLATION MODELS

Linear state space models are useful for stability analysis and control system design. Here we develop models of the form:

$$\dot{x} = A x' + B u' \qquad\qquad (M10.24)$$

$$y' = C x' \qquad\qquad (M10.25)$$

where $'$ is used to represent the deviation variables, $x' = x - x_s$, $u' = u - u_s$ (the subscript s indicates the steady-state values). Defining

$$K_i = \frac{\partial y_i}{\partial x_i} = \frac{\alpha}{(1 + (\alpha - 1)x_i)^2} \tag{M10.26}$$

and linearizing the dynamic equations (M10.13)–(M10.17)

$$A_{1,1} = \frac{\partial f_1}{\partial x_1} = -\frac{V_R}{M_D} \tag{M10.27}$$

$$A_{1,2} = \frac{\partial f_1}{\partial x_2} = \frac{V_R K_2}{M_D} \tag{M10.28}$$

For $i = 2$ to $NF - 1$:

$$A_{i,i-1} = \frac{\partial f_i}{\partial x_{i-1}} = \frac{L_R}{M_T} \tag{M10.29}$$

$$A_{i,i} = \frac{\partial f_i}{\partial x_i} = -\left(\frac{L_R + V_R K_i}{M_T}\right) \tag{M10.30}$$

$$A_{i,i+1} = \frac{\partial f_i}{\partial x_{i+1}} = \frac{V_R K_{i+1}}{M_T} \tag{M10.31}$$

For the feed stage:

$$A_{NF,NF-1} = \frac{\partial f_{NF}}{\partial x_{NF-1}} = \frac{L_R}{M_T} \tag{M10.32}$$

$$A_{NF,NF} = \frac{\partial f_{NF}}{\partial x_{NF}} = -\left(\frac{L_S + V_R K_i}{M_T}\right) \tag{M10.33}$$

$$A_{NF,NF+1} = \frac{\partial f_{NF}}{\partial x_{NF+1}} = \frac{V_S K_{NF+1}}{M_T} \tag{M10.34}$$

For $i = NF+1$ to $NS-1$:

$$A_{i,i-1} = \frac{\partial f_i}{\partial x_{i-1}} = \frac{L_S}{M_T} \tag{M10.35}$$

$$A_{i,i} = \frac{\partial f_i}{\partial x_i} = -\left(\frac{L_S + V_S K_i}{M_T}\right) \tag{M10.36}$$

$$A_{i,i+1} = \frac{\partial f_i}{\partial x_{i+1}} = \frac{V_S K_{i+1}}{M_T} \tag{M10.37}$$

and for the reboiler (stage NS)

$$A_{NS,NS-1} = \frac{\partial f_i}{\partial x_{i-1}} = \frac{l_{NS}}{M_B} \qquad\qquad\qquad \text{(M10.38)}$$

$$A_{NS,NS} = \frac{\partial f_i}{\partial x_i} = -\left(\frac{B + V_S K_{NS}}{M_B}\right) \qquad\qquad \text{(M10.39)}$$

Now, for the derivatives with respect to the inputs; $u_1 = L_R = L_1$ and $u_2 = V_S = V_{\text{reboiler}}$:

$$B_{1,1} = \frac{\partial f_1}{\partial u_1} = 0 \qquad\qquad B_{1,2} = \frac{\partial f_1}{\partial u_2} = 0 \qquad \text{(M10.40)}$$

For $i = 1$ to $NS-1$:

$$B_{i,1} = \frac{\partial f_1}{\partial u_1} = \frac{x_{i-1} - x_i}{M_T} \qquad\qquad B_{i,2} = \frac{\partial f_1}{\partial u_2} = \frac{y_{i+1} - y_i}{M_T} \qquad \text{(M10.41)}$$

and for the bottom stage:

$$B_{NS,1} = \frac{\partial f_1}{\partial u_1} = \frac{x_{i-1} - x_i}{M_{NS}} \qquad\qquad B_{NS,2} = \frac{\partial f_1}{\partial u_2} = \frac{x_{NS} - y_{NS}}{M_{NS}} \qquad \text{(M10.42)}$$

If the output variables are the overhead and bottoms compositions, then:

$$C_{1,1} = 1, \text{ while } C_{1,i} = 0 \text{ for } i \neq 1 \qquad\qquad \text{(M10.43)}$$

$$C_{2,NS} = 1, \text{ while } C_{1,i} = 0 \text{ for } i \neq 1 \qquad\qquad \text{(M10.44)}$$

M10.6.1   Transforming the State Space Linear Models to Transfer Function Form

The matrix transfer function is:

$$G(s) = C(sI - A)^{-1}B \qquad\qquad \text{(M10.45)}$$

It is easy to generate MATLAB m-files to calculate each of the state-space matrices (A,B,C) for a particular set of parameters (and steady-state compositions). For a column of reasonable size (say the 41-stage example) the denominator polynomial in (M10.45) would be quite large (say 41st order). What is often more useful is to be able to directly calculate the steady-state gain matrix, as shown below.

The steady-state gain matrix is:

$$G = -CA^{-1}B \qquad\qquad \text{(M10.46)}$$

where, again, it is easy to generate a MATLAB m-file to perform this calculation.

M10.7   MULTIPLICITY BEHAVIOR

Even simple ideal binary distillation columns have been shown recently to have interesting steady-state and dynamic behavior, including multiple steady-states. Nice examples are shown by Jacobsen and Skogestad (1991, 1994). The key assumption that must be made for this behavior to occur is that mass flows, rather than molar flows, are manipu-

lated. The reader is encouraged to read these papers and modify the MATLAB m-files presented in this chapter to illustrate the behavior shown by Jacobsen and Skogestad.

SUMMARY

In this chapter we have developed modeling equations to describe the steady-state and dynamic behavior of ideal, binary distillation columns. The 41-stage column example shows that steady-state distillate and bottom compositions are a nonlinear function of the manipulated inputs (distillate and vapor boil-up flows). Also, the dynamic responses of these compositions depends on the magnitude and direction of changes in the manipulated inputs.

REFERENCES AND FURTHER READING

The following undergraduate chemical engineering texts develop the steady-state modeling equations for ideal binary distillation:

King, C.J. (1980). *Separations Processes.* 2nd ed. New York: McGraw-Hill.

McCabe, W.L., & J.C. Smith. (1976). *Unit Operations of Chemical Engineering,* 3rd ed. New York: McGraw-Hill.

The dynamic modeling equations for distillation are presented by:

Luyben, W.L. (1990). *Process Modeling, Simulation and Control for Chemical Engineers,* 2nd ed. New York: McGraw-Hill.

More advanced treatments of steady-state and dynamic distillation models are presented by:

Holland, C.D. (1981). *Fundamentals of Multicomponent Distillation.* New York: McGraw-Hill.

Holland, C.D., & A.I. Liapis. (1983). *Computer Methods for Solving Dynamic Separation Problems.* New York: McGraw-Hill.

The parameters for Example M10.1 are presented in the following two references:

Skogestad, S., & M. Morari. (1988). Understanding the dynamic behavior of distillation columns. *Ind. Eng. Chem. Res.,* 27(10): 1848-1862.

Morari, M., & E. Zafiriou. (1988). *Robust Process Control.* Englewood Cliffs, NJ: Prentice-Hall.

The possibility of multiple steady-state behavior in ideal binary distillation is presented by:

Jacobsen, E.W., & S. Skogestad. (1991). Multiple steady-states in ideal two-product distillation. *AIChE J.,* 37(4): 499-511.

Jacobsen, E.W., & S. Skogestad. (1994). Instability of distillation columns. *AIChE J.,* 40(9): 1466-1478.

STUDENT EXERCISES

1. Consider a simple 1 tray (3 stage) column with the overhead condenser as stage 1, the feed tray as stage 2 and the reboiler as stage 3. Use the following parameters and inputs:

α = 5
R = 3 mol/min
q_F = 1
F = 1 mol/min
D = 0.5 mol/min
z_F = 0.5 mole fraction of light component

Find the bottoms product flowrate, the stripping section flowrate and the vapor boil-up rate (stripping section vapor flowrate). Use `fsolve` and `dist_ss.m` to find the resulting compositions:

$$x = \begin{bmatrix} 0.703 \\ 0.486 \\ 0.297 \end{bmatrix} = \begin{bmatrix} \text{distillate composition} \\ \text{composition of stage 2 (the feed tray)} \\ \text{bottoms product composition} \end{bmatrix}$$

Consider now the dynamic behavior, with the initial conditions of the stage compositions equal to the steady-state solution. The additional parameters needed for the dynamic simulation are the molar holdups on each stage. Use:

M_1 = M_D = overhead receiver molar holdup = 5 mol
M_2 = feed tray molar holdup = 0.5 mol.
M_3 = 5 = bottoms (reboiler) molar holdup = 5 mol

At time zero, the reflux is changed from 3.0 mol/min to 3.2 mol/min. Use `ode45` and `dist_dyn.m` to simulate the dynamic behavior shown in the figures below.
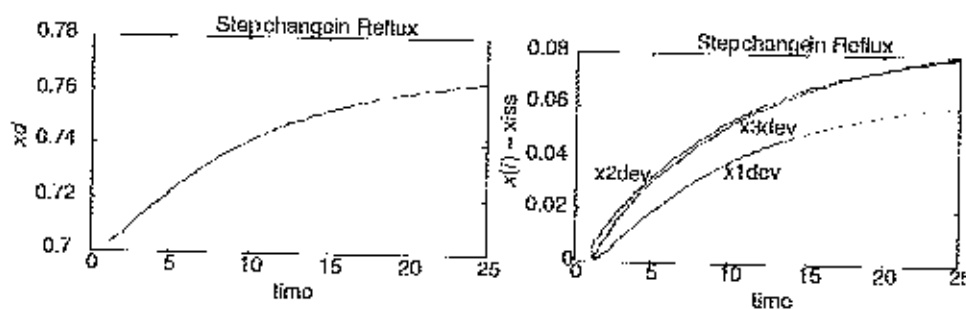
The Reflux is step changed from 3.0 to 3.2 at $t = 1$ minute.

APPENDIX

dist_ss.m

```
function f = dist_ss(x);
%
% solve for the steady-state stage compositons in an ideal
% binary distillation column using fsolve.
%
% (c) 1993 B. Wayne Bequette - 21 june 93
% revised 31 Dec 96
%
% All flowrates are molar quantities.  Stages are numbered
% from the top down.  A total condenser is assumed.
% The overhead receiver is stage 1.  The partial reboiler
% is stage ns (the number of equilibrium "trays" is then
% ns-1).  The column parameters should be specified in the
% DIST_PAR array.
%
% to use this function, enter the following in the command
% window, or from a script file (after defining parameters
% in the DIST_PAR array:
%
% x = fsolve('dist_ss',x0)
%
% where x0 is a vector of initial guesses for the liquid
% phase stage compositions (length(x0) = ns)
%
   global DIST_PAR
%
% DIST_PAR is a vector of distillation column parameters
%         used by both dist_ss.m and dist_dyn.m
%
   if length(DIST_PAR) < 8;
     disp('not enough parameters given in DIST_PAR')
       disp(' ')
       disp('check to see that global DIST_PAR has been defined')
       return
   end
%
   alpha   = DIST_PAR(1);   % relative volatility (2.5)
   ns      = DIST_PAR(2);   % total number of stages (3)
   nf      = DIST_PAR(3);   % feed stage (2)
   feed    = DIST_PAR(4);   % feed flowrate (1)
   zfeed   = DIST_PAR(5);   % feed composition, light comp (0.5)
   qf      = DIST_PAR(6);   % feed quality (1 = sat'd liqd,
%                               0 = sat'd vapor) (1)
   reflux  = DIST_PAR(7);   % reflux flowrate (3)
   vapor   = DIST_PAR(8);   % reboiler vapor flowrate (3.5)
%
% DIST_PAR(9:19) used by dist_dyn.m (distillation dynamics)
%  dist      = distillate product flowrate
```

```
%    f(i)        - ith comp mat bal equation
%    lbot        = bottoms product flowrate
%    lr          = liquid flow in rectifying section (top)
%    ls          - liquid flow in stripping section (bottom)
%    vr          = vapor flow - rectifying sec (= vapor + feed*(1 qf)
%    vs          - vapor flow - stripping section (- vapor)
%    x(i)        - mole frac light component on stage i, liq
%    y(i)        - mole frac light component on stage i, vap
%
% rectifying and stripping section liquid flowrates
%
     lr      =    reflux;
     ls      -    reflux + feed*qf;
%
% rectifying and stripping section vapor flowrates
%
     vs      =    vapor;
     vr      =    vs +   feed*(1-qf);
%
% distillate and bottoms rates
%
     dist    -    vr - reflux;
     lbot    =    ls - vs;
%
     if dist < 0
        disp('error in specifications, distillate flow < 0')
        return
      end
      if lbot < 0
        disp('error in specifications, stripping section ')
        disp(' ')
        disp('liquid flowrate is negative')
        return
      end
%
% zero the function vector
%
     f = zeros(ns,1);
%
% calculate the equilibrium vapor compositions
%
     for i=1:ns;
       y(i)-(alpha*x(i))/(1.+(alpha-1.)*x(i));
     end
%
% material balances
%
% overhead receiver
%
     f(1)-(vr*y(2) (dist+reflux)*x(1));
%
% rectifying (top) section
```

```
%
        for i=2:nf-1;
          f(i)=lr*x(i-1)+vr*y(i+1)-lr*x(i)-vr*y(i);
        end
%
% feed stage
%
        f(nf)  =   lr*x(nf-1)+vs*y(nf+1)-ls*x(nf)-
                   vr*y(nf)+feed*zfeed;
%
% stripping (bottom) section
%
        for i=nf+1:ns-1;
          f(i)=ls*x(i-1)+vs*y(i+1)-ls*x(i)-vs*y(i);
        end
%
% reboiler
%
        f(ns)=(ls*x(ns-1)-lbot*x(ns)-vs*y(ns));
```

dist_dyn.m

```
  function xdot = dist_dyn(t,x);
%
% solve for the transient stage compositions in an ideal
% binary distillation column using ode45.
%
% (c) 1997 B. Wayne Bequette - 24 Jan 1997
% revised 31 Dec 96
%
% All flowrates are molar quantities.  Stages are numbered
% from the top down.  A total condenser is assumed.
% The overhead receiver is stage 1.  The partial reboiler
% is stage ns (the number of equilibrium "trays" is then
% ns-1). The column parameters should be specified in the
% DIST_PAR array.
%
% to use this function, enter the following in the command
% window, or from a script file (after defining parameters
% in the DIST_PAR array:
%
% [t,x] = ode45('dist_dyn',t0,tf,x0)
%
% where x0 is a vector of initial values for the liquid
% phase stage compositions (length(x0) - ns)
%
  global DIST_PAR
%
% DIST_PAR is a vector of distillation column parameters
%          used by both dist_ss.m and dist_dyn.m
```

```
%
   if length(DIST_PAR) < 11;
     disp('not enough parameters given in DIST_PAR')
       disp(' ')
       disp('check to see that global DIST_PAR has been defined')
       return
   end
%
   alpha     = DIST_PAR(1);    % relative volatility (1.5)
   ns        = DIST_PAR(2);    % total number of stages (41)
   nf        = DIST_PAR(3);    % feed stage (21)
   feedi     = DIST_PAR(4);    % initial feed flowrate (1)
   zfeedi    = DIST_PAR(5);    % initial feed composition, light comp
                                 (0.5)
   qf        = DIST_PAR(6);    % feed quality (1 = sat'd liqd,
%                                   0 = sat'd vapor) (1)
   refluxi   = DIST_PAR(7);    % initial reflux flowrate (2.706)
   vapori    = DIST_PAR(8);    % initial reboiler vapor flowrate
                                 (3.206)
   md        = DIST_PAR(9);    % distillate molar hold-up (5)
   mb        = DIST_PAR(10);   % bottoms molar hold-up (5)
   mt        = DIST_PAR(11);   % stage molar hold-up (0.5)
%
   if length(DIST_PAR) == 19;
     stepr   = DIST_PAR(12);  % magnitude step in reflux (0)
     tstepr  = DIST_PAR(13);  % time of reflux step change (0)
     stepv   = DIST_PAR(14);  % magnitude step in vapor (0)
     tstepv  = DIST_PAR(15);  % time of vapor step change (0)
     stepzf  = DIST_PAR(16);  % magnitude of feed comp change (0)
     tstepzf = DIST_PAR(17);  % time of feed comp change (0)
     stepf   = DIST_PAR(18);  % magnitude of feed flow change (0)
     tstepf  = DIST_PAR(19);  % time of feed flow change (0)
   else
     stepr = 0; tstepr = 0; stepv = 0; tstepv = 0;
     stepzf = 0; tstepzf = 0; stepf = 0; tstepf = 0;
   end
%
% DIST_PAR(9:19) used by dist_dyn.m (distillation dynamics)
%  dist      = distillate product flowrate
%  lbot      = bottoms product flowrate
%  lr        = liquid flow in rectifying section (top)
%  ls        = liquid flow in stripping section (bottom)
%  vr        = vapor flow - rectifying sec (= vapor + feed*(1-qf)
%  vs        = vapor flow - stripping section (= vapor)
%  x(i)      = mole frac light component on stage i, liq
%  xdot(i)   = light component ith stage mat bal equation
%  y(i)      = mole frac light component on stage i, vap
%
%  check disturbances in reflux, vapor boil-up, feed composition
%       and feed flowrate
%
   if t < tstepr;
```

```
        reflux = refluxi;
      else
        reflux = refluxi + stepr;
      end
%
    if t < tstepv;
      vapor = vapori;
    else
      vapor = vapori + stepv;
    end
%
    if t < tstepzf;
      zfeed = zfeedi;
    else
      zfeed = zfeedi + stepzf;
    end
%
    if t < tstepf;
      feed = feedi;
    else
      feed = feedi + stepf;
    end
%
% rectifying and stripping section liquid flowrates
      lr      =   reflux;
      ls      =   reflux + feed*qf;
%
% rectifying and stripping section vapor flowrates
%
      vs      =   vapor;
      vr      =   vs +  feed*(1-qf);
%
% distillate and bottoms rates
%
      dist    = vr - reflux;
      lbot    =   ls - vs;
%
      if dist < 0
          disp('error in specifications, distillate flow < 0')
          return
        end
        if lbot < 0
          disp('error in specifications, stripping section ')
          disp(' ')
          disp('liquid flowrate is negative')
          return
        end
%
% zero the function vector
%
      xdot = zeros(ns,1);
%
```

```
% calculate the equilibrium vapor compositions
%
        for i=1:ns;
          y(i)=(alpha*x(i))/(1.+(alpha-1.)*x(i));
        end
%
% material balances
%
% overhead receiver
%
        xdot(1)=(1/md)*(vr*y(2)-(dist+reflux)*x(1));
%
% rectifying (top) section
%
        for i=2:nf-1;
          xdot(i)=(1/mt)*(lr*x(i-1)+vr*y(i+1)-lr*x(i)-vr*y(i));
        end
%
% feed stage
%
        xdot(nt)   = (1/mt)*(lr*x(nf-1)+vs*y(nf+1) ls*x(nf)-
          r*y(nt)+feed*zfeed);
%
% stripping (bottom) section
%
        for i=nf+1:ns-1;
          xdot(i)=(1/mt)*(ls*x(i-1)+vs*y(i+1) ls*x(i)-vs*y(i));
        end
%
% reboiler
%
        xdot(ns)=(1/mb)*(ls*x(ns-1) lbot*x(ns)-vs*y(ns));
```