ODEs are defined as VDOT, VCDOT, VTDOT, and TJDOT. At each point in
time, integration gives values for \( V, VC, VT, \) and \( TJ \). Then \( C_A \) and \( T \) are found
by dividing \( VC \) and \( VT \) by \( V \).

Figures 5.4 through 5.6 give results for disturbances in feed composition
and feed flow rate. Note that in Fig. 5.5 the controller gain has been decreased to
2.5 and a larger feed composition disturbance has been made. The response is quite oscillatory. We will discuss the tuning of temperature controllers in this
type of system in much more detail later in this book.

5.4 BINARY DISTILLATION COLUMN

The digital simulation of a distillation column is fairly straightforward. The main
complication is the large number of ODEs and algebraic equations that must be solved. We will illustrate the procedure first with the simplified binary distillation
column for which we developed the equations in Chap. 3 (Sec. 3.11). Equimolal
overflow, constant relative volatility, and theoretical plates have been assumed.
There are two ODEs per tray (a total continuity equation and a light component
continuity equation) and two algebraic equations per tray (a vapor-liquid phase
equilibrium relationship and a liquid-hydraulic relationship).

\[
\frac{dM_n}{dt} = L_{n+1} - L_n \tag{5.29}
\]

\[
\frac{d[M_n x_n]}{dt} = L_{n+1} x_{n+1} + V y_{n-1} - L_n x_n - V y_n \tag{5.30}
\]

\[
y_n = \frac{a x_n}{1 + (a - 1) x_n} \tag{5.31}
\]

\[
L_n = \bar{L}_n + \frac{M_n - \bar{M}_n}{\beta} \tag{5.32}
\]

Equation (5.32) is a simple linear relationship between the liquid holdup on a
tray, \( M_n \), and the liquid flow rate leaving the tray, \( L_n \). The parameter \( \beta \) is the
hydraulic time constant, typically 3 to 6 seconds per tray.

Since there are many trays and most are described by Eqs. (5.29) through
(5.32), it is logical to use “dimensioned” variables and to evaluate derivatives and
integrate using FORTRAN “DO” loops. It also makes sense to use a SUB-
ROUTINE or FUNCTION to find \( y_n \), given \( x_n \), because the same equation is
used over and over again.

At each instant in time we know all holdups \( M_n \) and all liquid compositions
\( x_n \). Our simulation logic is:

1. Calculate vapor compositions on all trays from Eq. (5.31).
2. Calculate all liquid flow rates from Eq. (5.32).
3. Evaluate all derivatives. These are the right-hand sides of Eqs. (5.29) and (5.30)
applied to all trays. These derivatives are called MDOT(N) and MXDOT(N)
in the program given in Table 5.7.
4. Integrate with Euler all ODEs and start again at step 1 above.
TABLE 4.7

Binary distillation column dynamics

C
C ASSUMPTIONS: CONSTANT RELATIVE VOLATILITY, EQUIMOLAL
C OVERFLOW, THEORETICAL TRAYS, SIMPLE LIQUID TRAY
C HYDRAULICS
C FEEDBACK CONTROLLERS MANIPULATE \( R \) AND \( V \) TO CONTROL \( X_D \) AND \( X_B \)
C DISTURBANCE IS A FEED COMPOSITION CHANGE FROM 0.50 TO 0.55
C AT TIME EQUAL ZERO
C
C DIMENSION X(20),Y(20),L(20),LO(20),M(20)
C DIMENSION MX(20),MDOT(20),MXDOT(20)
C REAL L,LO,M,MR,MX,MDOT,MXDOTT,MDO,MQ,MBO,KCD,KCB
C USE A FUNCTION STATEMENT FOR VLE
C EQUIL(XX)=ALPHA*XX/(1.+(ALPHA-1.)*XX)
C INITIAL CONDITIONS AND PARAMETER VALUES
C DATA NT,NF,MDO,MBO,MQ,MRO,VO,F,BETA,ALPHA/20,10,100,100.,
C + 10,0.388,0.178,0.1,100.0,1.2./
C DATA XR,XD/0.02,0.05,0.0719,0.08885,0.1318,0.18622,0.24651,
C + 0.3168,0.37948,0.43391,0.47688,0.51526,0.56295,0.61890,0.65852,
C + 0.70434,0.76019,0.85503,0.89995,0.91484,0.93408,0.96079,0.98/
C DATA KCD,KCB,TAUD,TAUB,DELTA,TIME,TPRINT,ERINTD,ERINTB/
C + 1,000.,1000.,5.,1,25.,.005,4e0.0/
C DISTURBANCE
C
C Z=0.55
C WRITE(6,1) Z,F
1 FORMAT(7X,'*=',F10.5,*,F=*,F10.2)
C INITIAL CONDITIONS
C DO 3 N=1,NT
C M(N)=MO
C MX(N)=M(N)+X(N)
C LO(N)=RO+F
C IF(N.GT.NF) LO(N)=RO
3 CONTINUE
C WRITE(6,2)
2 FORMAT(6X,TIME,FXB,XD,R,V*)
C TRAY LIQUID HYDRAULICS AND VLE
C 100 DO 20 N=1,NT
C Y(N)=EQUIL(X(N))
C L(N)=LO(N)+(M(N)-MO)/BETA
20 CONTINUE
C YB=EQUIL(XR)
C TWO PI FEEDBACK CONTROLLERS
C ERRB=62-XB
C ERRD=98-XD
C V+VO-KCB=(ERRB+ERINTB/TAUB)
C R+RO+KCD=(ERRD+ERINTD/TAUD)
C PERFECT LEVEL CONTROLLERS IN REFLUX DRUM AND COLUMN BASE
C D=V,R
C B=1(1)-V
C IF(R.LT.0.) GO TO 500
C IF(V.LT.0.) GO TO 500
C IF(D.LT.0.) GO TO 500
C IF(B.LT.0.) GO TO 500
C EVALUATE DERIVATIVES
C XDOT=(L(1)-X(1)-V*YB-B*XB)/MBO
C MDOT(1)=L(2)-L(1)
C MXDOTT(1)=V+(YB-B*Y(1))*(L(2)*X(2)-L(1)*X(1))
C DO 30 N=2,NF-1
TABLE 5.7 (continued)

C FEED PLATE

MDOT(N)=L(N+1)-L(N)
80 MXDOT(N)=V*(Y(N+1)-Y(N))+L(N+1)*X(N+1)-L(N)*X(N)
C MXDOT(N)=V*(Y(N+1)-Y(N))+L(N+1)*X(N+1)-L(N)*X(N)
DO 40 N=N+1,NT-1
40 MXDOT(N)=V*(Y(N+1)-Y(N))+L(N+1)*X(N+1)-L(N)*X(N)
MDOT(N)=L(N+1)-L(N)
MDOT(N)=L(N+1)-L(N)
MXT(N)=V*(Y(N+1)-Y(N))+L(N+1)*X(N+1)-L(N)*X(N)
XDDOT=V*(Y(N+1)-V(DT))/MDT
IF(TIME.LT.TPRINT) GO TO 50
WRITE(6,441)TIME,XB,X(10),XD,R,V
TPRINT=TPRINT+5
50 CONTINUE
C EULER INTEGRATION

TIME=TIME+DTFLTA
XB=XB+DELTA*XBDO T
DO 60 N=1,NT
M(N)=M(N)-MDOT(N)*DELTA
MX(N)=MX(N)+MXDOT(N)*DELTA
X(N)=MX(N)/M(N)
IF(X(N).LT.0) GO TO 500
IF(X(N).LT.1) GO TO 500
60 CONTINUE
XD=XD+XDDOT*DELTA
ERINT=ERINT+FRD*DELTA
ERINT=ERINT+FRD*DELTA
IF(TIME.LE.10) GO TO 100
STOP
500 WRITE(6,501)
501 FORMAT(‘LEVEL TOO LOW OR COMPOSITION UNREAL’)
STOP
END

Results

\[
\begin{align*}
Z &= 0.55000 \\
F &= 100.00
\end{align*}
\]

<table>
<thead>
<tr>
<th>TIME</th>
<th>XB</th>
<th>X10</th>
<th>XD</th>
<th>R</th>
<th>V</th>
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<td>0.08000</td>
<td>128.01</td>
<td>178.01</td>
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<td>0.02014</td>
<td>0.51325</td>
<td>0.08000</td>
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<td>0.52435</td>
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<tr>
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<tr>
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<tr>
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<tr>
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<tr>
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<td>0.52207</td>
<td>0.08016</td>
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<td>0.08029</td>
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<td>127.15</td>
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<td>0.08028</td>
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<td>182.47</td>
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</tbody>
</table>
It is very important to note that all derivatives are evaluated using the current values of all variables before integrating any of the ODEs. A fairly common mistake is to evaluate one derivative and to integrate that ODE before going on to the next ODE. This procedure is not correct and will lead to inaccurate answers.

We will assume constant holdups in the reflux drum \( M_D \) and in the column base \( M_B \). Proportional-integral feedback controllers at both ends of the column will change the reflux flow rate \( R \) and the vapor boilup \( V \) to control overhead composition \( x_D \) and bottoms composition \( x_B \) at setpoint values of 0.98 and 0.02 respectively.

Table 5.7 gives the program, the initial conditions, and the printed output results for a step change in feed composition from 0.50 to 0.55 at time equal zero.

5.5 MULTICOMPONENT DISTILLATION COLUMN

The extension of the simple ideal binary system considered in the preceding section to a nonideal multicomponent column is not difficult. The only changes that have to be made to the basic structure of the solution algorithm are:

1. More ordinary differential equations must be added per tray. We need one per component per tray. But this is easily programmed using doubly dimensioned variables \( X(N, J) \), where \( N \) is the tray number and \( J \) is the component number.

2. One energy balance per tray must be included if equimolar overflow cannot be assumed.

3. An appropriate multicomponent bubblepoint subroutine must be used. This may be a little more complex because of nonidealities, but as far as the main program is concerned, the bubblepoint subroutine is provided with known liquid compositions and a known pressure, and its job is to calculate the temperature and vapor compositions.

The general model was developed in Sec. 3.12. Table 5.8 gives a fairly general program for continuous multicomponent distillation.

The specific column simulated is assumed to have the following equipment configurations and conditions:

1. There is one feed plate onto which vapor feed and liquid feed are introduced.
2. Pressure is constant and known on each tray. It varies linearly up the column from \( P_B \) in the base to \( P_D \) at the top (psia).
3. Coolant and steam dynamics are negligible in the condenser and reboiler.
4. Vapor and liquid products \( D_v \) and \( D_L \) are taken off the reflux drum and are in equilibrium. Dynamics of the vapor space in the reflux drum and throughout the column are negligible.