Chapter 2 Numerical Methods with MATLAB

Linear Systems

2.1 In the photosynthesis reaction, water reacts with carbon dioxide to give glucose and oxygen. This reaction can be expressed as

$$x_1 CO_2 + x_2 H_2O \rightarrow x_3 O_2 + x_4 C_6 H_{12} O_6$$

Determine the values of coefficients x_1, x_2, x_3, and x_4 to balance the equation. Is it possible to determine these values? If not, under what conditions can the solutions be found?

2.1(Solution)

Carbon balance: $x_1 = 6x_4$, oxygen balance: $2x_1 + x_2 = 2x_3 + 6x_4$, hydrogen balance: $2x_2 = 12x_4$. Rearrangement of these equations gives

$$\begin{bmatrix} 1 & 0 & 0 & -6 \\ 2 & 1 & -2 & -6 \\ 0 & 2 & 0 & -12 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

We can use the backslash operator to get the solution:

```
>> x = A\b
x =
     0
     0
     0
     0
```

The given equations can be rewritten as

$$x_1 - 6x_4 = 0, x_2 - 6x_4 = 0, \; x_3 - 6x_4 = 0 \quad \Rightarrow \quad x_1 = 6x_4, x_2 = 6x_4, x_3 = 6x_4$$

Thus if we set $x_4 = 1$, we have $x_1 = x_2 = x_3 = 6$.

2.2 Four reactors are connected by pipes where directions of flow are depicted by means of arrows as shown in Figure P2.2[18]. The flow rate of the key component is given by the volumetric flow rate Q $(liter/sec)$ multiplied by the concentration C $(g/liter)$ of the component. The incoming flow rate is assumed to be equal to the outgoing rate. Using the flow rates given below, calculate the concentration at each reactor:

$$Q_{13} = 75\, liter/sec, \quad Q_{24} = 20\, liter/sec, \quad Q_{33} = 60\, liter/sec,$$
$$Q_{21} = 25\, liter/sec, \quad Q_{32} = 45\, liter/sec, \quad Q_{43} = 30\, liter/sec$$

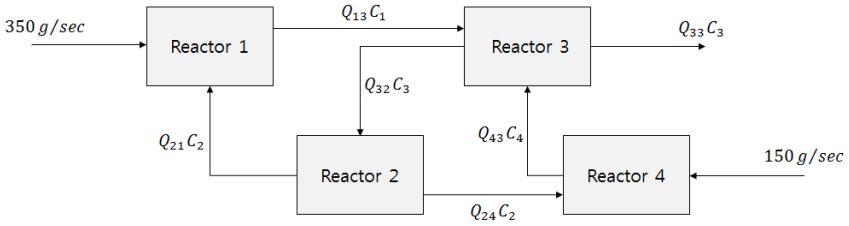

FIGURE P2.2

2.2(Solution)

Material balance for each reactor can be expressed as follows:

Reactor 1: $350 + Q_{21}C_2 = Q_{13}C_1 \Rightarrow 350 + 25C_2 = 75C_1 \Rightarrow 75C_1 - 25C_2 = 350$

Reactor 2: $Q_{32}C_3 = Q_{21}C_2 + Q_{24}C_2 \Rightarrow 45C_3 = 25C_2 + 20C_2 \Rightarrow 45C_3 - 45C_2 = 0$

Reactor 3:

$Q_{13}C_1 + Q_{43}C_4 = Q_{32}C_3 + Q_{33}C_3 \Rightarrow 75C_1 + 30C_4 = 45C_3 + 60C_3 \Rightarrow 75C_1 + 30C_4 - 105C_3 = 0$

Reactor 4: $150 + Q_{24}C_2 = Q_{43}C_4 \Rightarrow 150 + 20C_2 = 30C_4 \Rightarrow 30C_4 - 20C_2 = 150$

These equations can be rearranged as

$75C_1 - 25C_2 = 350, \quad -45C_2 + 45C_3 = 0, \quad 75C_1 - 105C_3 + 30C_4 = 0, \quad -20C_2 + 30C_4 = 150$

The following commands produce desired outputs:

```
>> A = [75 -25 0 0;0 -45 45 0;75 0 -105 30;0 -20 0 30]; b = [350 0 0 150]'; C = A\b
C =
    7.4444
    8.3333
    8.3333
   10.5556
```

2.3 Paraxylene, styrene, toluene and benzene are to be separated with the array of distillation columns shown in Figure P2.3.[19] Determine the molar flow rates ($kgmol/min$) of D_1, D_2, B_1, and B_2.

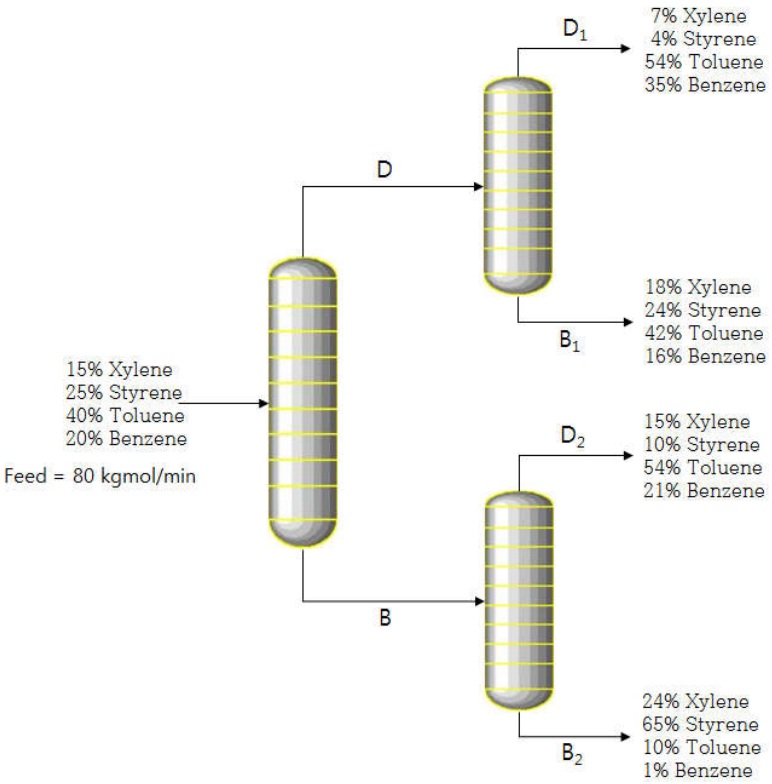

FIGURE P2.3

2.3(Solution)

Material balance for each component is given by:

Xylene: $0.07D_1 + 0.18B_1 + 0.15D_2 + 0.24B_2 = 0.15 \times 80 = 12$

Styrene : $0.04D_1 + 0.24B_1 + 0.1D_2 + 0.65B_2 = 0.25 \times 80 = 20$

Toluene : $0.54D_1 + 0.42B_1 + 0.54D_2 + 0.1B_2 = 0.4 \times 80 = 32$

Benzene : $0.35D_1 + 0.16B_1 + 0.21D_2 + 0.01B_2 = 0.2 \times 80 = 16$

These equations can be rearranged as $Ax = b$, which can be solved by using the backslash operator:

```
>> A = [0.07 0.18 0.15 0.24; 0.04 0.24 0.1 0.65;...
      0.54 0.42 0.54 0.1; 0.35 0.16 0.21 0.01];
>> b = [12 20 32 16]'; x = A\b
x =
    30.0000
    20.0000
    10.0000
    20.0000
```

We can see that D_1=30 kgmol/min, B_1=20 kgmol/min, D_2=10 kgmol/min, and B_2=20 kgmol/min.

2.4 Figure P2.4 shows a flat square plate the sides of which are held at constant temperatures (200℃ and 500℃). Find the temperatures at inner nodes (i.e., $T_7 - T_9$, $T_{12} - T_{14}$, $T_{17} - T_{19}$). The temperature at each inner node is assumed to be given by the average of temperatures of adjacent nodes.

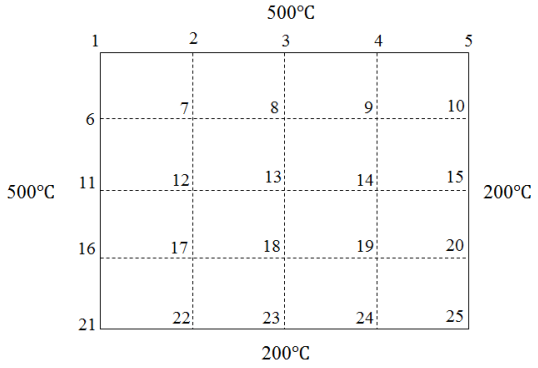

FIGURE P2.4

2.4(Solution)

The energy balance for each inner node should be set. For example, the energy balance for node 7 can be written as

$$q_7 = \frac{kA}{\Delta x}(T_6 - T_7) + \frac{kA}{\Delta x}(T_8 - T_7) + \frac{kA}{\Delta y}(T_{12} - T_7) + \frac{kA}{\Delta y}(T_2 - T_7)$$

where $\Delta x = \Delta y$. Dividing both sides by kA and rearranging, we have

$$\frac{q_7}{kA} = T_8 + T_{12} - 4T_7 + 1000$$

At steady-state, the heat sink(q_7/kA) becomes zero. Energy balance for each inner node can be represented as follows:

$T_1 = T_2 = T_3 = T_4 = T_6 = T_{11} = T_{16} = 500$ ℃, $T_{10} = T_{15} = T_{20} = T_{25} = T_{24} = T_{23} = T_{22} = 200$ ℃

$T_5 = \frac{500 + 200}{2} = 350$ ℃, $T_{21} = \frac{500 + 200}{2} = 350$ ℃

Node 7: $-4T_7 + T_8 + T_{12} = -1000$

Node 8: $-4T_8 + T_7 + T_{13} + T_9 = -500$

Node 9: $-4T_9 + T_8 + T_{14} = -700$

Node 12: $-4T_{12} + T_{13} + T_{17} + T_7 = -500$

Node 13: $-4T_{13} + T_{12} + T_{14} + T_{18} + T_8 = 0$

Node 14: $-4T_{14} + T_{13} + T_{19} + T_9 = -200$

Node 17: $-4T_{17} + T_{18} + T_{12} = -700$

Node 18: $-4T_{18} + T_{17} + T_{19} + T_{13} = -200$

Node 19: $-4T_{19} + T_{18} + T_{14} = -400$

These equations can be rearranged in vector-matrix form as:

$$\text{Ax} = \text{b} \Rightarrow \begin{bmatrix} -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -4 & 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -4 & 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & -4 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & -4 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & -4 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & -4 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & -4 \end{bmatrix} \begin{bmatrix} T_7 \\ T_8 \\ T_9 \\ T_{12} \\ T_{13} \\ T_{14} \\ T_{17} \\ T_{18} \\ T_{19} \end{bmatrix} = \begin{bmatrix} -1000 \\ -500 \\ -700 \\ -500 \\ 0 \\ -200 \\ -700 \\ -200 \\ -400 \end{bmatrix}$$

We can use the backslash operator to find solutions:

```
>> A = [-4 1 0 1 0 0 0 0 0;1 -4 1 0 1 0 0 0 0; 0 1 -4 0 0 1 0 0 0;1 0 0 -4 1 0 1 0 0;...
        0 1 0 1 -4 1 0 1 0;0 0 1 0 1 -4 0 0 1; 0 0 0 1 0 0 -4 1 0;0 0 0 0 1 0 1 -4 1;...
        0 0 0 0 0 1 0 1 -4];
>> b = [10 5 7 5 0 2 7 2 4]'*(-100); T = A\b
T =
   457.1429
   414.2857
   350.0000
   414.2857
   350.0000
   285.7143
   350.0000
   285.7143
   242.8571
```

2.5 Figure P2.5 shows an ideal multi-component flash drum. The feed mixture of flow rate F consists of three isomers of xylene: o-xylene(1), m-xylene(2) and p-xylene(3). The feed contains mole fractions z_i of each component at temperature T_f and pressure P_f. In the flash drum, vapor-liquid equilibrium is achieved at T and P with a liquid flow rate L and vapor flow rate V. The vapor pressure of each component is assumed to be represented by Antoine equation given by

$$\log_{10} P_i^{sat}(mmHg) = A_i - \frac{B_i}{T(^\circ\text{C}) + C_i}$$

where A_i, B_i and C_i are the Antoine coefficients for species i. Table P2.5 lists the Antoine coefficients for three isomers of xylene. Assume that $P = 760\ mmHg$, $F = 1\ mol/sec$ and $L = 0.2\ mol/sec$. Generate a plot showing the range of operating temperature T as a function of the mole fraction of o-xylene $z_1 (0.1 \le z_1 \le 0.9)$.[20]

TABLE P2.5
Antoine Coefficients for Three Isomers of Xylene

Component	A_i	B_i	C_i	Boiling point(℃)
o-xylene(1)	6.99891	1474.679	213.69	144.4
m-xylene(2)	7.00908	1462.266	215.11	139.1
p-xylene(3)	6.99052	1453.430	215.31	138.4

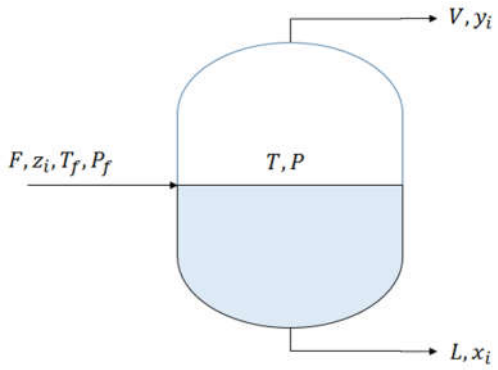

FIGURE P2.5 Illustration of ideal multi-component flash drum.

2.5(Solution)

From mass balance and equilibrium relationship, we can get the following linear equations:

$$x_i P_i^{sat} = y_i P \quad (i = 1,2,3), \quad x_1 L + y_1 V = z_1 F, \quad \sum_{i=1}^{3} x_i = \sum_{i=1}^{3} y_i = 1$$

Since $\mathrm{F} = 1\ \mathrm{mol/s}$ and $\mathrm{L} = 0.2\ \mathrm{mol/s}$, $\mathrm{V} = \mathrm{F} - \mathrm{L} = 0.8\ \mathrm{mol/s}$. Rearrangement of these equations gives the following linear system:

$$\begin{bmatrix} P_1^{sat} & 0 & 0 & -P & 0 & 0 \\ 0 & P_2^{sat} & 0 & 0 & -P & 0 \\ 0 & 0 & P_3^{sat} & 0 & 0 & -P \\ L & 0 & 0 & V & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ z_1 F \\ 1 \\ 1 \end{bmatrix}$$

where $\mathrm{x}_4 = \mathrm{y}_1, \mathrm{x}_5 = \mathrm{y}_2$ and $\mathrm{x}_6 = \mathrm{y}_3$. For $0.1 \le \mathrm{z}_1 \le 0.9$, the script flashrange.m uses the backslash operator(\) to solve the linear system for $0.1 \le \mathrm{z}_1 \le 0.9$, checks the constraints $\sum_{\mathrm{i}=1}^{3} \mathrm{x}_\mathrm{i} = \sum_{\mathrm{i}=1}^{3} \mathrm{y}_\mathrm{i} = \sum_{\mathrm{i}=1}^{3} \mathrm{z}_\mathrm{i} = 1$, determines the possible operating temperature range ($\mathrm{T}_{\min} \le \mathrm{T} \le \mathrm{T}_{\max}$), and plots T vs. z.

```
% flashrange.m
clear all;
z = 0.1:0.01:0.9; n = length(z); % feed composition of o-xylene
Tl = zeros(1,n); Th = zeros(1,n);
for k = 1:n
    [Tmin Tmax] = eqflash(z(k)); Tl(k) = Tmin; Th(k) = Tmax;
end
plot(z,Th,z,Tl,'--'), grid, xlabel('z_1'), ylabel('T(deg.C)')
legend('T_{max}','T_{min}','location','best')

function [Tmin Tmax] = eqflash(z)
nT = 500; Tl = 138.4; Th = 144.4; T = linspace(Tl,Th,nT); flnd = 0;
for k = 1:nT
    [x,y,zv] = compxyz(T(k),z);
    if sum(x>0) == 3 && sum(y>0) == 3 && sum(zv>0) == 3
        if flnd == 0, Tmin = T(k); flnd = 1; end
    else
        if flnd == 1, Tmax = T(k-1); return; end
    end
end
end

function [x,y,zv] = compxyz(T,z)
```

```
A = [6.99891 7.00908 6.99052]; B = [1474.679 1462.266 1453.430]; C = [213.69 215.11 215.31];
F = 1; L = 0.2; V = F - L; P = 760; % operating condition
zv(1) = z; Pv = 10.^(A - B./(T + C)); % vapor pressure by Antoine eqn.
Am = [Pv(1) 0 0 -P 0 0; 0 Pv(2) 0 0 -P 0; 0 0 Pv(3) 0 0 -P;L 0 0 V 0 0;...
        1 1 1 0 0 0;0 0 0 1 1 1]; % coefficient matrix of linear system
b = [0 0 0 z*F 1 1]'; % right-hand side of linear system
s = Am\b; x = s(1:3); y = s(4:6);
for k = 2:3, zv(k) = x(k)*L + y(k)*V; end
end
```

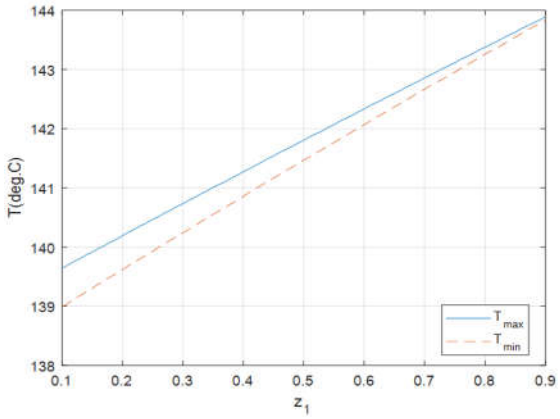

FIGURE P2.5(S) Operating temperature range.

2.6 Consider the simplified process flow diagram shown in Figure P2.6.[21] In the flow diagram, m_i $(i = 1,2,\cdots,12)$ represents flow rate of stream i. Assume that no mass accumulations and chemical reactions take place in the process units. The feed flow m_1 is maintained at $100\ kg/min$, $m_3 = 0.7m_1 - m_2, m_6 = (m_7 + m_8)/3.2$, $m_7 = 0.84m_{12} - m_4$, $m_8 = 0.2m_5$, $m_{10} = 0.2m_9$, $m_9 = 0.85m_2 - m_{11}$, and $m_{12} = 0.55m_1 - m_9$. It is required to determine the flow rates m_i $(i = 2,3,\cdots,12)$.

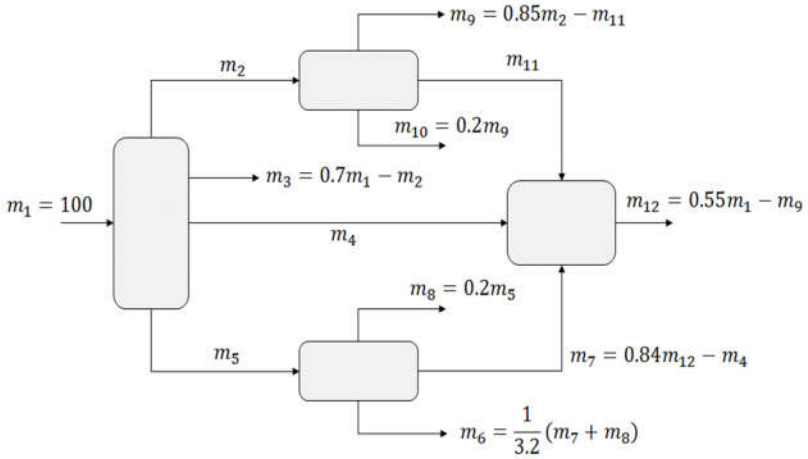

FIGURE P2.6 Simplified process flow diagram.

2.6(Solution)
Since there are no chemical reactions and mass accumulations, we can easily set up mass balance for each process unit as follows:

$$m_2 + m_3 + m_4 + m_5 = m_1 = 100, \quad m_2 = m_9 + m_{10} + m_{11}, \quad m_5 = m_6 + m_7 + m_8,$$
$$m_4 + m_7 + m_{11} = m_{12}$$

Rearrangement of the process specifications gives

$$m_2 + m_3 = 0.7m_1 = 70, \quad 3.2m_6 - m_7 - m_8 = 0, \quad m_7 + m_4 - 0.84m_{12} = 0,$$
$$m_5 - 5m_8 = 0, \quad m_9 - 5m_{10} = 0, \quad 0.85m_2 - m_9 - m_{11} = 0, \quad m_9 + m_{12} = 0.55m_1 = 55$$

These linear equations can be rewritten in terms of matrix and vectors as follows:

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & -1 & -1 & 0 \\ 0 & 0 & 0 & 1 & -1 & -1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & -1 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3.2 & -1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -0.84 \\ 0 & 0 & 0 & 1 & 0 & 0 & -5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -5 & 0 & 0 \\ 0.85 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} m_2 \\ m_3 \\ m_4 \\ m_5 \\ m_6 \\ m_7 \\ m_8 \\ m_9 \\ m_{10} \\ m_{11} \\ m_{12} \end{bmatrix} = \begin{bmatrix} 100 \\ 0 \\ 0 \\ 0 \\ 70 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 55 \end{bmatrix}$$

The script flowmass.m defines the linear system and uses the backslash operator(\) to find the solution.

```
% flowmass.m
A = zeros(11,11); A(1,1) = 1; A(1,2) = 1; A(1,3) = 1; A(1,4) = 1;
A(2,1) = 1; A(2,8) = -1; A(2,9) = -1; A(2,10) = -1;
A(3,4) = 1; A(3,5) = -1; A(3,6) = -1; A(3,7) = -1;
A(4,3) = 1; A(4,6) = 1; A(4,10) = 1; A(4,11) = -1;
A(5,1) = 1; A(5,2) = 1; A(6,5) = 3.2; A(6,6) = -1; A(6,7) = -1;
A(7,3) = 1; A(7,6) = 1; A(7,11) = -0.84;
A(8,4) = 1; A(8,7) = -5; A(9,8) = 1; A(9,9) = -5;
A(10,1) = 0.85; A(10,8) = -1; A(10,10) = -1; A(11,8) = 1; A(11,11) = 1;
b = zeros(11,1); b(1,1) = 100; b(5,1) = 70; b(11,1) = 55; % right-hand side of the linear system
m = A\b; m = m' % use backslash operator to solve the linear system

>> flowmass
m =
40.0   30.0   9.4565   20.5435   4.8913   11.5435   4.1087   30.0   6.0   4.0   25.0
```

2.7 The process shown in Figure P2.7 consists of a reactor and a separator. The reactants A and B are fed into the reactor with flow rates A_1 and B_1, respectively. The following two reactions are taking place in the reactor:

Reaction 1: $A + B \rightarrow C$ (extent of reaction = ξ_1)

Reaction 2: $A + C \rightarrow D$ (extent of reaction = ξ_2)

The intermediate product C produced by the *Reaction 1* needs to be converted to the desired product D by *Reaction 2*. The single-pass conversion of the reactor is 90% with a 30% selectivity for *Reaction 2*. In the separator, the flow B_2 is evenly split between the product stream (stream 3) and the recycle stream (stream 4), 65% of D and 85% of C fed into the separator are recycled through stream 4, and 10% of flow A_2 is lost to the product stream (stream 3).[22]

The feed flow rates are $A_1 = 10\ mol/sec$ and $B_1 = 20\ mol/sec$. Determine flow rates A_i, B_i, C_i, D_i $(i = 2,3,4)$ and extents of reaction ξ_1 and ξ_2 for *Reaction 1* and *2*.

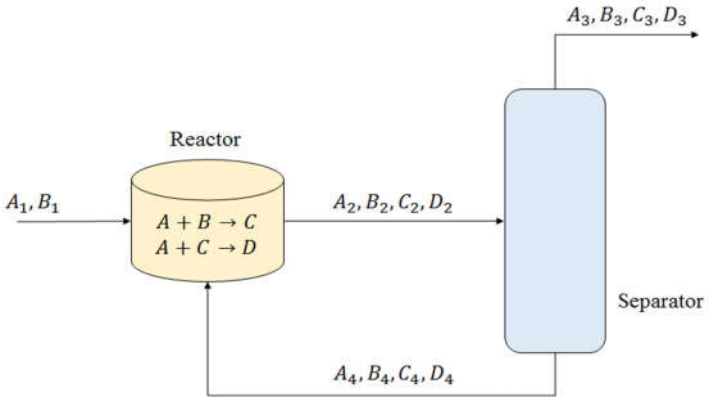

FIGURE P2.7 A process consisting of a reactor and a separator with recycle.

2.7(Solution)

The steady-state mass balances on the reactor are as follows:

$$-A_2 + A_4 - \xi_1 - \xi_2 = -A_1, \quad -B_2 + B_4 - \xi_1 = -B_1$$
$$-C_2 + C_4 + \xi_1 - \xi_2 = 0, \quad -D_2 + D_4 + \xi_2 = 0$$

The mass balances for the separator are:

$$A_2 - A_3 - A_4 = 0, \quad B_2 - B_3 - B_4 = 0, \quad C_2 - C_3 - C_4 = 0, \quad D_2 - D_3 - D_4 = 0$$

From the conversion and selectivity of the reaction, we have

$$-0.9A_4 + \xi_1 + \xi_2 = 0.9A_1, \quad 0.3\xi_1 - 0.7\xi_2 = 0$$

The separator specifications give

$$-0.65D_2 + D_4 = 0, \quad B_3 - B_4 = 0, \quad 0.1A_2 - A_3 = 0, \quad 0.85C_2 - C_4 = 0$$

Let $x_1 = A_2, x_2 = B_2, x_3 = C_2, x_4 = D_2$, $x_5 = A_3, x_6 = B_3, x_7 = C_3$, $x_8 = D_3$, $x_9 = A_4$, $x_{10} = B_4$, $x_{11} = C_4, x_{12} = D_4, x_{13} = \xi_1$ and $x_{14} = \xi_2$. Then the mass balances can be represented in terms of matrix and vectors as follows:

-1	0	0	0	0	0	0	0	1	0	0	0	-1	-1
0	-1	0	0	0	0	0	0	0	1	0	0	-1	0
0	0	-1	0	0	0	0	0	0	0	1	0	1	-1
0	0	0	-1	0	0	0	0	0	0	0	1	0	1
1	0	0	0	-1	0	0	0	-1	0	0	0	0	0
0	1	0	0	0	-1	0	0	0	-1	0	0	0	0
0	0	1	0	0	0	-1	0	0	0	-1	0	0	0
0	0	0	1	0	0	0	-1	0	0	0	-1	0	0
0	0	0	0	0	0	0	0	-0.9	0	0	0	1	1
0	0	0	0	0	1	0	0	0	-1	0	0	0	0
0	0	0.85	0	0	0	0	0	0	0	-1	0	0	0
0	0	0	-0.65	0	0	0	0	0	0	0	1	0	0
0.1	0	0	0	-1	0	0	0	0	0	0	0	0	0

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -0.3 & 0.7 \end{bmatrix}$$

$$\times \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \\ x_7 \\ x_8 \\ x_9 \\ x_{10} \\ x_{11} \\ x_{12} \\ x_{13} \\ x_{14} \end{bmatrix} = \begin{bmatrix} -10 \\ -20 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 9 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

The script *rxtsep* defines the linear system and uses the backslash operator(\) to find the solution.

```
% rxtsep.m: reactor and separator with recycle
A = zeros(14,14); A(1,1) = -1; A(1,9) = 1; A(1,13) = -1; A(1,14) = -1;
A(2,2) = -1; A(2,10) = 1; A(2,13) = -1; A(3,3) = -1; A(3,11) = 1; A(3,13) = 1; A(3,14) = -1;
A(4,4) = -1; A(4,12) = 1; A(4,14) = 1; A(5,1) = 1; A(5,5) = -1; A(5,9) = -1;
A(6,2) = 1; A(6,6) = -1; A(6,10) = -1; A(7,3) = 1; A(7,7) = -1; A(7,11) = -1;
A(8,4) = 1; A(8,8) = -1; A(8,12) = -1; A(9,9) = -0.9; A(9,13) = 1; A(9,14) = 1;
A(10,6) = 1; A(10,10) = -1; A(11,3) = 0.85; A(11,11) = -1;
A(12,4) = -0.65; A(12,12) = 1; A(13,1) = 0.1; A(13,5) = -1;
A(14,13) = -0.3; A(14,14) = 0.7;
b = zeros(14,1); b(1,1) = -10; b(2,1) = -20; % right-hand side vector
x = A\b; x = x' % solve the linear system using backslash operator

>> rxtsep
x =
    10.9890 27.5385 23.7363 7.6295 1.0989 13.7692 3.5604 2.6703 9.8901 13.7692 20.1758
    4.9592 6.2308 2.6703
```

We can see that
$A_2 = 10.989, B_2 = 27.5385, C_2 = 23.7363, D_2 = 7.6295$, $A_3 = 1.0989, B_3 = 13.7692$, $C_3 = 3.5604$, $D_3 = 2.6703$, $A_4 = 9.8901$, $B_4 = 13.7692$, $C_4 = 20.1758$, $D_4 = 4.9592$, $\xi_1 = 6.2308$, and $\xi_2 = 2.6703$.

Nonlinear Equations

2.8 The volume fraction of red blood cells in blood is called hematocrit. The core region hematocrit (H_c) is given by

$$\frac{H_c}{H_0} = 1 + \frac{(1-\sigma^2)^2}{\sigma^2\{2(1-\sigma^2) + \sigma^2(1-\alpha H_c)\}}, \qquad \sigma = 1 - \frac{\delta}{R}, \qquad \alpha = 0.07 \exp\left(2.49 H_c + \frac{1107}{T} e^{-1.69 H_c}\right)$$

where

H_0 is the hematocrit at inlet of blood vessel
$\delta(\mu m)$ is the thickness of the plasma layer
$R(\mu m)$ is the radius of the blood vessel
$T(K)$ is the temperature

Find H_c if $\delta = 2.94\ \mu m$, $R = 16\ \mu m$, $T = 315\ K$, and $H_0 = 0.45$.

2.8(Solution)

```
% hemat.m: determination of volume fraction of red blood cells in blood (hematocrit)
clear all;
delta = 2.94; R = 16; T = 315; H0 = 0.45; % data
s = 1 - delta/R; s2 = s^2;
f = @(x) [1+(1-s2)^2/(s2*(2*(1-s2)+s2*(1-x*0.07*exp(2.49*x+1107*exp(-1.69*x)/T)))) - x/H0];
x0 = H0/2; Hc = fzero(f,x0)

>> hemat
Hc =
    0.5296
```

2.9 The total number of unbound receptors present on a cell surface at equilibrium is given by

$$\frac{R_t}{R_{eq}} = 1 + \nu\left(\frac{L_0}{K_D}\right)(1 + K_x R_{eq})^{f-1}$$

where

R_t is the total number of receptors present on the cell surface
R_{eq} is the equilibrium concentration of unbound receptors present on the cell surface
ν is the number of binding sites
L_0 is the ligand concentration
K_D is the dissociation constant
K_x is the crosslinking equilibrium constant
f is the total number of binding sites available for binding to a single cell

Determine the equilibrium concentration R_{eq} using the data given below.

Data: $R_t = 10692,\ \nu = 17,\ L_0 = 2.1 \times 10^{-9}\ M,\ K_D = 7.76 \times 10^{-5}\ M,\ K_x = 5.82 \times 10^{-5},\ f = 9.$

2.9(Solution)

```
% recept.m: determine the number of unbounded receptors
clear all;
Rt = 10692; nu = 17; L0 = 2.1e-9; Kd = 7.76e-5; Kx = 5.82e-5; n = 9; % data
f = @(x) [1 + nu*(L0/Kd)*(1 + Kx*x)^(n-1) - Rt/x];
x0 = Rt; Req = fzero(f,x0)

>> recept
Req =
    1.0475e+04
```

2.10 The vapor pressure (mmHg) of *n*-pentane (A) and *n*-hexane (B) can be calculated from the Antoine equation (T:℃)[23]:

$$\log P_A = 6.85221 - \frac{1064.63}{T + 232.0}, \qquad \log P_B = 6.87776 - \frac{1171.53}{T + 224.366}$$

(1) Calculate the bubble point temperature and equilibrium composition associated with a liquid mixture of 10 mol % *n*-pentane and 90 mol % *n*-hexane at 1 atm.

(2) Repeat the calculations for liquid mixtures containing 0 mol % up to 100 mol % of *n*-pentane. Plot the bubble point temperature and mol % of *n*-pentane in the vapor phase as a function of the mol % in the liquid phase.

2.10(Solution)

At dew point, the sum of the partial pressure of each component should be equal to the total pressure (1 atm): $x_A P_A + x_B P_B = 760\ \ mmHg$