

Scilab Textbook Companion for
Elements Of Chemical Reaction
Engineering(copy)
by H. S. Fogler¹

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May 24, 2016

¹Funded by a grant from the National Mission on Education through ICT, <http://spoken-tutorial.org/NMEICT-Intro>. This Textbook Companion and Scilab codes written in it can be downloaded from the "Textbook Companion Project" section at the website <http://scilab.in>

Book Description

Title: Elements Of Chemical Reaction Engineering(copy)

Author: H. S. Fogler

Publisher: Prentice Hall International Inc., New Jersey

Edition: 3

Year: 2009

ISBN: 0-13-973785-5

Scilab numbering policy used in this document and the relation to the above book.

Exa Example (Solved example)

Eqn Equation (Particular equation of the above book)

AP Appendix to Example(Scilab Code that is an Appednix to a particular Example of the above book)

For example, Exa 3.51 means solved example 3.51 of this book. Sec 2.3 means a scilab code whose theory is explained in Section 2.3 of the book.

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Chapter 1

Mole Balances

check Appendix [AP 9](#) for dependency:

10_3.sci

Scilab code Exa 1.3 clear

```
1 //clear//
2 clc
3 clear
4 exec("1.3data.sci");
5
6 //CA = 0.1*CA0;
7 V = (v0/k)*log(1/0.1);
8 disp("V =")
9 disp(V)
10 disp ("dm^3")
```

Chapter 2

Conversion and Reactor Sizing

check Appendix [AP 47](#) for dependency:

2_1.sci

Scilab code Exa 2.1 clear

```
1 //clear//
2 clc
3 clear
4 exec("2.1 data . sci");
5 CA0=(yA0*P0)/(R*T0);
6 FA0 = CA0*v0;
7 disp("CA0 =")
8 disp(CA0)
9 disp (" mol/dm^3")
10 disp("FA0 =")
11 disp(FA0)
12 disp(" mol/s")
```

check Appendix [AP 46](#) for dependency:

2_2.sci

Scilab code Exa 2.2 clear

```
1 //clear//
2 clc
3 clear
4 exec("2.2 data . sci");
5 CA0=(yA0*P0)/(R*T0);
6 FA0 = CA0*v0;
7 V = FA0*X*(1/-rA)
8
9 disp("FA0 =")
10 disp(FA0)
11 disp("mol/s")
12 disp("V =")
13 disp(V)
14 disp ("dm^3")
```

check Appendix [AP 45](#) for dependency:

2_3.sci

Scilab code Exa 2.3 clear

```
1 //clear//
2 clc
3 clear
4 exec("2.3 data . sci");
5 CA0=(yA0*P0)/(R*T0);
6 FA0 = CA0*v0;
7 //V = FA0*X*(1/-rA)
8
9 V = FA0*inttrap(X,p)
10 disp("FA0 =")
11 disp(FA0)
12 disp("mol/s")
13 disp("V =")
```

```
14 disp(V)
15 disp ("dm^3")
16 disp("Answer is slightly different from the book
      because inttrap command of SCILAB uses
      trapezoidal integration, while in book it has
      been calculated using five point formulae.")
```

check Appendix [AP 44](#) for dependency:

2_4.sci

Scilab code Exa 2.4 clear

```
1 //clear//
2 clc
3 clear
4 exec("2.4data.sci");
5
6
7 VCSTR = FA0*X(7)*(1/-rAat);
8 VPFR = FA0*inttrap(X,p)
9 disp("VCSTR =")
10 disp(VCSTR)
11 disp("dm^3")
12 disp("VPFR =")
13 disp(VPFR)
14 disp ("dm^3")
```

check Appendix [AP 43](#) for dependency:

2_5.sci

Scilab code Exa 2.5 clear

```

1 //clear//
2 clc
3 clear
4 exec("2.5data.sci");
5
6
7 V1 = FA0*X1*(1/-rA);
8 V2 = FA0*(X2-X1)*(1/-rA2);
9 V = FA0*X*(1/-rA2);
10 disp("V1 =")
11 disp(V1)
12 disp("dm^3")
13 disp("V2 =")
14 disp(V2)
15 disp("dm^3")
16 disp("V =")
17 disp(V)
18 disp("dm^3")

```

check Appendix [AP 42](#) for dependency:

2_6.sce

Scilab code Exa 2.6 clear

```

1 //clear//
2 clc
3 clear all
4 exec("2.6data.sci");
5
6
7 X1 = X(1:5);
8 p1 = p(1:5);
9 V1 = FA0*inttrap(X1,p1)
10 X2 = X(5:9);
11 p2 = p(5:9);

```

```

12 V2 = FA0*inttrap(X2,p2)
13 V=V1+V2;
14 disp("V1 =")
15 disp(V1)
16 disp("dm^3")
17 disp("V2 =")
18 disp(V2)
19 disp ("dm^3")
20 disp("V =")
21 disp(V)
22 disp ("dm^3")

```

check Appendix [AP 41](#) for dependency:

2_7.sci

Scilab code Exa 2.7 clear

```

1 //clear//
2 clc
3 clear
4 exec("2.7data.sci");
5
6
7 X = X(1:6);
8 p = p(1:6);
9 V1 = FA0*inttrap(X,p);
10 V2 = FA0*(X2-X1)*(1/-rA2);
11 V=V1+V2;
12 disp("V1 =")
13 disp(V1)
14 disp("dm^3")
15 disp("V2 =")
16 disp(V2)
17 disp ("dm^3")
18 disp("V =")

```

```
19 disp(V)
20 disp("dm^3")
```

Chapter 3

Rate Laws and Stoichiometry

check Appendix [AP 40](#) for dependency:

3_5.sci

Scilab code Exa 3.5 clear

```
1 //clear//
2 clc
3 clear
4 exec("3.5 data . sci");
5 CD=CA0*(X/3);
6 CB=CA0*((CB0/CA0)-(X/3));
7 CD1=CA0*(X1/3);
8 CB1=CA0*((CB0/CA0)-(X1/3));
9 disp("For 20% conversion")
10 disp("CD =")
11 disp(CD)
12 disp (" mol/dm^3")
13 disp("CB =")
14 disp(CB)
15 disp(" mol/dm^3")
16 disp("For 90% conversion")
17 disp("CD =")
```

```
18 disp(CD1)
19 disp (" mol/dm3")
20 disp ("CB =")
21 disp(CB1)
22 disp (" mol/dm3")
```

Chapter 4

Isothermal Reactor Design

check Appendix [AP 39](#) for dependency:

4_1.sci

Scilab code Exa 4.1 clear

```
1 //clear//
2 clc
3 clear
4 exec("4.1 data . sci");
5
6 x=t;
7 y =((CA0-CC)/CA0);
8
9 yi=interp1n([x;y],x);
10 plot2d(x,y,logflag='nl');
11
12 k = log(y(9)/y(2))/(t(9)-t(2));
13
14
15 disp("k =")
16 disp(k)
17 disp ("min^-1")
```

check Appendix [AP 36](#) for dependency:

4_2.sci

Scilab code Exa 4.2 clear

```
1 //clear//
2 clc
3 clear
4 exec("4.2 data . sci");
5
6 FA0 = FC/X;
7 vA0 = FA0/CA01;
8 vB0 = vA0;
9 v0 = vA0+vB0;
10 V = v0*X/(k*(1-X));
11
12 // CSTR in parallel
13 V1 = 800/7.48;
14
15 Tau =V1/(v0/2);
16 Da= Tau*k;
17 Xparallel = Da/(1+Da)
18
19 // CSTR in series
20 Tau =V1/v0;
21 n=2;
22 Xseries = 1- (1/(1+Tau*k)^n);
23
24 disp("Reactor volume")
25 disp(V)
26 disp ("ft ^3")
27 disp("CSTR in parallel X =")
28 disp(Xparallel)
29 disp("CSTR in series X =")
```

30 `disp(Xseries)`

check Appendix [AP 35](#) for dependency:

4_4.sci

Scilab code Exa 4.4 clear

```
1 //clear//
2 clc
3 clear
4 exec("4.4data.sci");
5
6 FA0 = FB/X;
7 CA0 = yA0*P0/(R*T0);
8 R = 1.987;
9 k2 = k1*exp((E/R)*((1/T1)-(1/T2)));
10 V = (FA0/(k2*CA0))*((1+e)*log(1/(1-X))-e*X);
11
12 disp("Reactor volume")
13 disp(V)
14 disp("ft^3")
```

check Appendix [AP 34](#) for dependency:

4_5.sci

Scilab code Exa 4.5 clear

```
1 //clear//
2 clc
3 clear
4 exec("4.5data.sci");
5
```

```

6 G = m/Ac;
7 bita0 = (G*(1-phi)/(gc*rho*Dp*phi^3))*((150*(1-phi)*
    mu/Dp)+1.75*G);
8 bita0 = bita0/(144*14.7); //atm/ft
9 P = ((1-(2*bita0*L/P0))^0.5)*P0;
10 deltaP = P0 - P;
11
12 disp(" deltaP")
13 disp(deltaP)
14 disp(" atm")

```

check Appendix [AP 33](#) for dependency:

4_6.sci

Scilab code Exa 4.6 clear

```

1 //clear//
2 clc
3 clear
4 exec(" 4.6 data . sci");
5
6 FT0 = FA0+FB0+FI;
7 yA0 = FA0/FT0;
8 e = yA0*(1-.5-1);
9 PA0 = yA0*P0;
10 kdes = k*PA0*(1/2)^(2/3);
11 alpha = 2*bita0/(Ac*(1-phi)*rhoc*P0);
12 W = (1 - (1-(3*alpha*FA0/(2*kdes))*((1+e)*log(1/(1-X
    ))-e*X))^(2/3))/alpha;
13
14
15 disp("W")
16 disp(W)
17 disp("lb of catalyst per tube")

```

check Appendix [AP 32](#) for dependency:

4_7.sci

Scilab code Exa 4.7 clear

```
1 //clear//
2 clc
3 clear
4 exec("4.7data.sci");
5 W = 0:1:60;
6 function w=f(W,Y)
7
8 w=zeros(2,1);
9 w(1)= (kprime/FA0)*((1-Y(1))/(1+e*Y(1)))*Y(2);
10 w(2) = -alpha*(1+e*Y(1))/(2*Y(2));
11 endfunction
12
13
14 x=ode([0;1],W0,W,f);
15 for i= 1:61
16     F(i) = (1+e*x(1,i))/x(2,i);
17 end
18 F= F';
19 for i= 1:61
20     rate(i) = (kprime)*((1-x(1,i))/(1+e*x(1,i)))*x(2,i
21     );
21 end
22 rate =rate';
23
24 scf(1)
25 plot2d(W,rate);
26 xtitle('Figure E4-7.1 Reaction rate porfile down
27     the PBR', 'w', 'rate' );
27 scf(2)
28
```

```

29 l1=x(1,: )'
30 l2=x(2,: )'
31 l3=F'
32 plot2d(W',[l1 l2 l3]);
33
34 xtitle( 'Figure E4-7.2 ', 'w', 'x,y,z' ) ;
35 legend(['x';'y';'f']);

```

check Appendix [AP 31](#) for dependency:

4_8.sci

Scilab code Exa 4.8 clear

```

1 //clear//
2 clc
3 clear
4 exec("4.8 data . sci");
5 Z = 0:1:12;
6 function w=f(Z,Y)
7
8 w=zeros(2,1);
9 Ac= 3.14*((R^2)-(Z-L)^2);
10 Ca = Ca0*(1-Y(1))*Y(2)/(1+Y(1));
11 ra =kprime*Ca*rhocat*(1-phi);
12 G= m/Ac;
13 V =3.14*(Z*(R^2)-(1.3*(Z-L)^3)-(1/3)*L^3)
14 bita = (98.87*G+25630*G^2)*0.01;
15 W=rhocat*(1-phi)*V
16 w(1)= -ra*Ac/FA0
17 w(2) = -bita/P0/(Y(2)*(1+Y(1)));
18 endfunction
19
20
21 x=ode([0;1],Z0,Z,f);
22 for i= 1:length(Z)

```

```

23     V(1,i) =3.14*Z(1,i)*((R^2)-(Z(1,i)-L)^2)
24     W1(1,i)=rhocat*(1-phi)*V(1,i)
25 end
26
27 l1=x(1,:)';
28 l2=x(2,:)';
29
30 plot2d(W1',[l1 l2]);
31
32 xtitle('Figure E4-8.2','w','x,y');
33 legend(['x';'y']);

```

check Appendix [AP 30](#) for dependency:

4_9.sci

Scilab code Exa 4.9 clear

```

1 //clear//
2 clc
3 clear
4 exec("4.9data.sci");
5 V = 0:1:100;
6 function w=f(V,fa)
7
8     w=zeros(1,1);
9     ft =2*(fa0-fa(1))
10    Ca = Ct0*fa(1)/ft;
11    fb = 2*(fa0-fa(1));
12    Cb = Ct0*fb/ft;
13    w(1)= -ka*(Ca-(Cb^2)/kc)
14
15 endfunction
16
17
18 x=ode([9.99],V0,V,f);

```

```

19
20 for i= 1:101
21     fb(1,i) = 2*(fa0-x(1,i));
22 end
23 l1=x';
24 l2=fb';
25
26 plot2d(V',[l1 l2]);
27
28 xtitle('Figure E4-9.1 Molar flow rate profiles', 'V
        ', 'fa,fb' );
29 legend(['fa'; 'fb']);

```

check Appendix [AP 38](#) for dependency:

4__10.sci

Scilab code Exa 4.10 clear

```

1 //clear//
2 clc
3 clear
4 exec("4__10.sci");
5 V = 0:1:500;
6 function w=f(V,F)
7
8     w=zeros(3,1);
9
10    Ft=F(1)+F(2)+F(3);
11    ra = -k*Ct0*((F(1)/Ft)-(Ct0/kc)*(F(2)/Ft)*(F(3)/Ft)
        );
12    w(1)= ra;
13    w(2) = -ra-kc*Ct0*(F(2)/Ft)
14    w(3) = -ra;
15
16 endfunction

```



```

17
18
19 x=ode([10;0;0],V0,V,f);
20
21 l1=x(1,:)';
22 l2=x(2,:)';
23 l3=x(3,:)';
24 plot2d(V',[l1 l2 l3]);
25
26 xtitle('Figure E4-10.2', 'V', 'Fa,Fb,Fc' );
27 legend(['Fa';'Fb';'Fc']);

```

check Appendix [AP 37](#) for dependency:

4__11.sci

Scilab code Exa 4.11 clear

```

1 //clear//
2 clc
3 clear
4 exec("4__11.sci");
5 t = 0:1:500;
6 function w=f(t,C)
7
8 w =zeros(4,1);
9
10 v = v0+v00*t;
11 w(1)= -k*C(1)*C(2)-v00*C(1)/v;
12 w(2) = -k*C(1)*C(2)+v00*(Cb0-C(2))/v;
13 w(3) = k*C(1)*C(2)-v00*C(3)/v;
14 w(4) = k*C(1)*C(2)-v00*C(4)/v;
15
16 endfunction
17
18

```

```

19 x=ode([.049;0;0;0],t0,t,f);
20 l1=x(1,:)';
21 l2=x(2,:)';
22 l3=x(3,:)';
23 for i = 1:length(t)
24     rate(1,i)=k*x(1,i)*x(2,i)
25     end
26 scf(1)
27 plot2d(t',[l1 l2 l3]);
28
29 xtitle('Figure E4-11.1 Concentration-time
        trajectories ', 't', 'Ca,Cb,Cc' ) ;
30 legend(['Ca';'Cb';'Cc']);
31 scf(2)
32 plot2d(t,rate)
33 xtitle('Figure E4-11.2 Reaction rate-time
        trajectories ', 't', 'Reaction Rate(mols dm^3)' )
        ;
34
35
36
37
38 'V

```

Chapter 5

Collection and Analysis of Rate Data

Scilab code Exa 5.1 clear

```
1 //clear//
2 p = [ 1.44 .95 .74]';
3 dt = 2.5
4 t = [0 2.5 5]';
5 dp(1) = ( 3*p(1)+4p(2)-p(3))/(2*dt);
6 for i=2:n1
7   dp p(i+3
```

check Appendix [AP 29](#) for dependency:

5_2.sci

Scilab code Exa 5.2 clear

```
1 //clear//
2 clc
3 clear
```

```

4 exec(" 5.2 data . sci");
5 for i =1:length(t)
6 g(i) =log(2*P0/(3*P0-P(i)));
7 end
8 plot2d(t,g);
9
10 xtitle( 'Figure E4-11.2 Plot of processed data', 't
      (min)', '2PTo/3PTo-PT' ) ;

```

check Appendix [AP 28](#) for dependency:

5_3.sci

Scilab code Exa 5.3 clear

```

1 //Clear//
2 clc
3 clear
4 exec(" 5.3 data . sci");
5
6 x=log(CHCl);
7 y=log(-rHCl);
8 plot2d(x,y);
9
10 xtitle( 'Figure E5-3.2 ', 'CHCl (g mol/ liter)', '
      rHCl0 (g mol / cm^2.s)' ) ;

```

check Appendix [AP 26](#) for dependency:

4__4.sci

check Appendix [AP 27](#) for dependency:

5_4.sci

Scilab code Exa 5.4 clear

```
1 //Clear//
2 clc
3 clear
4 exec("5.4data.sci");
5
6 rCH4 = (v0/W)*CCH4;x
7 x=log(PCO);
8 y = log(rCH4)
9 alpha= (y(3)-y(2))/(x(3)-x(2));
10 //plot2d(x,y)
11 disp("alpha")
12 disp(alpha)
```

Chapter 6

Multiple Reactions

check Appendix [AP 25](#) for dependency:

6_6.sci

Scilab code Exa 6.6 clear

```
1 //Clear//
2 clc
3 clear
4 exec("6.6data.sci");
5 t = 0:.01:.5;
6 function w=f(t,c)
7
8 w =zeros(3,1);
9
10 r1 = -k1*c(2)*c(1)^.5;
11 r2 = -k2*c(3)*c(1)^.5;
12 w(1)= r1+r2;
13 w(2) = r1;
14 w(3) = -r1+r2;
15
16 endfunction
17
```

```

18 x=ode([.021;.0105;0],t0,t,f);
19
20 l1=x(1,:)';
21 l2=x(2,:)';
22 l3=x(3,:)';
23
24 plot2d(t',[l1 l2 l3]);
25
26 xtitle('Figure E6-6.1', 'Tau (hr)', 'Concentration
        (lb mol/ft^3)');
27 legend(['CH';'CM';'CX']);

```

check Appendix [AP 24](#) for dependency:

6_8.sci

Scilab code Exa 6.8 clear

```

1 //clear//
2 clc
3 clear
4 exec("6.8data.sci");
5 v = 0:.1:10;
6 function w =FF(v,f)
7
8 w =zeros(6,1);
9 ft = f(1)+f(2)+f(2)+f(4)+f(5)+f(6);
10 r1a = -5*8*(f(1)/ft)*(f(2)/ft)^2;
11 r2a = -2*4*(f(1)/ft)*(f(2)/ft);
12 r4c = -5*3.175*(f(3)/ft)*(f(1)/ft)^(2/3);
13 r3b = -10*8*((f(3)/ft)^2)*(f(2)/ft);
14 Ca =2*f(1)/ft;
15 Cb =2*f(2)/ft;
16 Cc =2*f(3)/ft;
17 Cd =2*f(4)/ft;
18 Ce =2*f(5)/ft;

```

```

19 Cf =2*f(6)/ft;
20 w(1)= 1.25*r1a+.75*r2a+r3b;
21 w(2) = r1a+r2a+2*r4c/3;
22 w(3) = -r1a+2*r3b+r4c;
23 w(4) =-1.5*r1a-1.5*r2a-r4c;
24 w(5) =.5*r2a-5*r4c/6;
25 w(6) = -2*r3b;
26
27 endfunction
28
29 x=ode([9;9;0;0;0;0],v0,v,FF);
30
31 plot2d(v,x(1,:)/10,rect=[1,0,10,1.5]); //B
32 plot2d(v,x(2,:)/10,rect=[1,0,10,1.5]); //A
33 plot2d(v,x(3,:)/10,rect=[1,0,10,1.5]); //C
34 plot2d(v,x(4,:)/10,rect=[1,0,10,1.5]);
35 plot2d(v,x(5,:)/10,rect=[1,0,10,1.5]);
36 plot2d(v,x(6,:)/10,rect=[1,0,10,1.5]);
37 xtitle('FigureE');
38 legend(['B';'A';'C';'D';'E';'F']);

```

Chapter 7

Nonelementary Reaction Kinetics

check Appendix [AP 23](#) for dependency:

7_7.sci

Scilab code Exa 7.7 clear

```
1 //clear//
2 clc
3 clear
4 exec("7.7data.sci");
5 for i=1:length(Curea)
6 x(i)= 1/Curea(i);
7 y(i) = 1/(-rurea(i));
8 end
9 slope = (y(5)-y(1))/(x(5)-x(1));
10 plot2d(x,y)
11
12 xtitle( 'Figure E7-7.1', '1/Curea', '1/-rurea' ) ;
13
14 disp("(Km/Vma = slope)")
15 disp(slope)
```

check Appendix [AP 22](#) for dependency:

7_8.sci

Scilab code Exa 7.8 clear

```
1 //clear//
2 clc
3 clear
4 exec("7.8data.sci");
5 Vmax = (Et2/Et1)*Vmax1
6 t = (Km/Vmax)*log(1/(1-X))+Curea0*X/Vmax;
7 disp("t")
8 disp(t)
9 disp("s")
```

check Appendix [AP 21](#) for dependency:

7_9.sci

Scilab code Exa 7.9 clear

```
1 //clear//
2 clc
3 clear
4 exec("7.9data.sci");
5 t = 0:.1:12;
6 function w=f(t,c)
7
8 w =zeros(3,1);
9
10 rd = c(1)*.01;
11 rsm = m/c(1);
```

```

12 kobs= (umax*(1-c(3)/93)^.52);
13 rg= kobs*c(1)*c(2)/(ks+c(2));
14 //r2 = -k2*c(3)*c(1)^.5;
15 w(1)= rg-rd;
16 w(2) = ysc*(-rg)-rsm;
17 w(3) = rg*ypc;
18
19 endfunction
20
21 x=ode([1;250;0],t0,t,f);
22
23 l1=x(1,:)';
24 l2=x(2,:)';
25 l3=x(3,:)';
26
27 plot2d(t',[l1 l2 l3]);
28
29 xtitle('Figure E7-9.1 concentrations as a function
         of time', 't (hr)', 'C (g/dm^3)') ;
30 legend(['Cc'; 'Cs'; 'Cp']);

```

Chapter 8

Steady State Nonisothermal Reactor Design

check Appendix [AP 18](#) for dependency:

8_3.sci

Scilab code Exa 8.3 clear

```
1 //clear//
2 clc
3 clear
4 exec("8.3data.sci");
5 deltaHRx0 = 2*H0NH3-3*H0H2-HN2;
6 deltaCp = 2*CpNH3-3*CpH2-CpN2;
7 deltaHRx = deltaHRx0+deltaCp*(T-TR);
8 disp("The heat of reaction on the basis on the moles
      of H2 reacted is =")
9 disp((1/3)*deltaHRx*4.184)
10 disp("J at 423 K")
```

check Appendix [AP 17](#) for dependency:

8_4.sci

Scilab code Exa 8.4 clear

```
1 //clear//
2 clc
3 clear
4 exec("8.4data.sci");
5 HRx0 = HOC-HOB-HOA;
6 deltaCp = CpC-CpB-CpA;
7 deltaHRx0 = HRx0+deltaCp*(TR-TR);
8 v0 = vA0+vB0+VM0;
9 tau = V/v0;
10 CA0 = FA0/v0;
11 phiM0 = FM0/FA0;
12 phiB0 = FB0/FA0;
13 Cpi = CpA+phiB0*CpB+phiM0*CpM;
14
15 for i =1:length(T)
16 XEB(i) = -Cpi*(T(i)-Ti0)/(deltaHRx0+deltaCp*(T(i)-TR
    ));
17 XMB(i) = tau*A*exp(-E/(R*T(i)))/(1+tau*A*exp(-E/(R*T
    (i))));
18 end
19
20
21
22 plot2d(T',[XEB XMB]);
23
24 xtitle('Figure E8-4.2', 'T(oR)', 'Conversion , X' )
    ;
25 legend(['XEB'; 'XMB']);
```

check Appendix [AP 16](#) for dependency:

8_6.sci

Scilab code Exa 8.6 clear

```
1 //clear//
2 clc
3 clear
4 exec("8.6 data . sci");
5 V = 0:.1:3.6;
6 function w=f(V,X)
7
8   w =zeros(1,1);
9   T =330+43.3*X;
10  k=31.1*exp(7906*(T-360)/(T*360));
11  Kc = 3.03*exp(-830.3*((T-360)/(T*360)));
12  Xe = Kc/(1+Kc);
13  ra = -k*Ca0*(1-(1+(1/Kc))*X);
14  w(1)= -ra/Fa0;
15  rate = -ra;
16 endfunction
17
18 x=ode([0],V0,V,f);
19
20 for i =1:length(x)
21   T(1,i) =330+43.3*x(1,i)
22
23   k(1,i)=31.1*exp(7906*(T(1,i)-360)/(T(1,i)*360));
24   Kc(1,i) = 3.03*exp(-830.3*((T(1,i)-360)/(T(1,i)
25     *360)));
26
27   ra(1,i) = k(1,i)*Ca0*(1-(1+(1/Kc(1,i)))*x(1,i));
28 end
29 scf(1)
30 plot2d(V,x(1,:));
31 xtitle('Figure E8-6.1a', 'V(m^3)', 'X' );
```

```

32 scf(2)
33 plot2d(V,T(1,:));
34
35 xtitle( 'Figure E8-6.1b', 'V(m^3)', 'T (K)' ) ;
36
37 scf(3)
38 plot2d(V,ra);
39
40 xtitle( 'Figure E8-6.1c', 'V(m^3)', '-ra (kmol/m^3hr
    )' ) ;

```

check Appendix [AP 15](#) for dependency:

8_8.sci

Scilab code Exa 8.7 clear

```

1 //clear//
2 clc
3 clear
4 exec("8.8data.sci");
5 for i = 1:length(T)
6     Xe(i) = 100000*exp(-33.78*(T(i)-298)/(T(i)))/(1+
7         100000*exp(-33.78*(T(i)-298)/T(i)));
8     XEB(i) = (2.5e-3)*(T(i)-300);
9 end
9 plot2d(T,[Xe XEB])
10
11 xtitle( 'Figure E8-8.1', 'T', 'X' ) ;
12 legend(['Xe';'XEB']);

```

Scilab code Exa 8.9 clear

```

1 //clear//
2 clc
3 clear
4 //eY(2)ec("8.6data.sci");
5 W = 0:1:28.58;
6 W0=0;
7 function w=f(W,Y)
8     w =zeros(3,1);
9
10
11 fao=.188
12 visc=.090
13 Ta=1264.67
14 deltah=-42471-1.563*(Y(3)-1260)+.00136*(Y(3)
        **2-1260**2)-(2.459*10**(-7))*(Y(3)**3-1260**3);
15 summ= 57.23+.014 * Y(3)-1.94 *10**(-6.)*Y(3)**2
16 dcp=-1.5625+2.72*10**(-3)*Y(3)-7.38*10**(-7)*Y(3)**2
17 k=360D*exp(-176008/Y(3)-(110.1*log(Y(3)))+912.8)
18 thetaso=0;
19 Po=2
20 Pao=.22
21 thetao=.91
22 eps=-.055
23 R=1.987;
24 Kp=exp(42311/R/Y(3)-11.24);
25 if(Y(2)<=.05)
26
27     ra=(-k*(.848-.012/(Kp**2)));
28 else
29     ra=(-k*(1-Y(2))/(thetaso+Y(2))**.5*(Y(1)/Po*Pao
        *((thetao-.5*Y(2))/((1+eps*Y(2)))-((thetaso+Y
        (2))/(1-Y(2)))**2/(Kp**2)));
30 end
31
32 w(1)=(-1.12*10**(-8)*(1-.055*Y(2))*Y(3))*(5500*visc
        +2288)/Y(1);
33 w(2)=-ra/fa0;
34 w(3)=(5.11*(Ta-Y(3))+(-ra)*(-deltah))/(fao*(summ+Y

```



```

        (2)*dcp))
35 endfunction
36
37 X=ode([2;0;1400],W0,W,f);
38
39 plot2d(W,X(1,:));
40 plot2d(W,X(3,:));

```

Scilab code Exa 8.10 clear

```

1 //clear//
2 clc
3 clear
4 //eY(2)ec("8.6 data . sci");
5 W = 0:1:28.58;
6 W0=0;
7 function w=f(W,Y)
8     w =zeros(3,1);
9
10
11 fao=.188
12 visc=.090
13 Ta=1264.67
14 deltah=-42471-1.563*(Y(3)-1260)+.00136*(Y(3)
        **2-1260**2)-(2.459*10**(-7))*(Y(3)**3-1260**3);
15 summ= 57.23+.014 * Y(3)-1.94 *10**(-6.)*Y(3)**2
16 dcp=-1.5625+2.72*10**(-3)*Y(3)-7.38*10**(-7)*Y(3)**2
17 k=360D*exp(-176008/Y(3)-(110.1*log(Y(3)))+912.8)
18 thetaso=0;
19 Po=2
20 Pao=.22
21 thetao=.91
22 eps=-.055
23 R=1.987;
24 Kp=exp(42311/R/Y(3)-11.24);

```

```

25 if(Y(2) < = .05)
26
27     ra=(-k*(.848-.012/(Kp**2)));
28 else
29     ra=(-k*(1-Y(2))/(thetaso+Y(2))**.5*(Y(1)/Po*Pao
        *((thetao-.5*Y(2))/((1+eps*Y(2)))-((thetaso+Y
        (2))/(1-Y(2))))**2/(Kp**2)));
30 end
31
32 w(1)=(-1.12*10**(-8)*(1-.055*Y(2))*Y(3))*(5500*visc
        +2288)/Y(1) ;
33 w(2)=-ra/fao ;
34 w(3)=(5.11*(Ta-Y(3))+(-ra)*(-deltah) )/(fao*(summ+Y
        (2)*dcp))
35 endfunction
36
37 X=ode([2;0;1400],W0,W,f);
38
39 plot2d(W,X(1,:));
40 plot2d(W,X(3,:));

```

check Appendix [AP 20](#) for dependency:

8__11.sci

Scilab code Exa 8.11 clear

```

1 //clear//
2 clc
3 clear
4 exec("8__11.sci");
5 V = 0:.01:1;
6
7 function w=f(V,Y)
8
9     w =zeros(4,1);

```

```

10
11 k1a=10*exp(4000*((1/300)-(1/Y(4))));
12 k2a=.09*exp(9000*((1/300)-(1/Y(4))))
13
14 Ft=Y(1)+Y(2)+Y(3);
15
16 Ca=Cto*(Y(1)/Ft)*(To/Y(4))
17 Cb=Cto*(Y(2)/Ft)*(To/Y(4))
18 Cc=Cto*(Y(3)/Ft)*(To/Y(4))
19 r1a=-k1a*Ca;
20 r2a=-k2a*Ca^2;
21
22 w(1)=r1a+r2a;
23 w(2)=-r1a;
24
25 w(3)=-r2a/2;
26 w(4)=(4000*(373-Y(4))+(-r1a)*20000+(-r2a)*60000)
    /(90*Y(1)+90*Y(2)+180*Y(3));
27 endfunction
28
29 x=ode([100;0;0;423],V0,V,f);
30
31 scf(1)
32 plot2d(V,x(4,:));
33
34 xtitle('Figure E8-11.1', 'V', 'T' );
35
36 scf(2)
37
38 l1=x(1,:)';
39 l2=x(2,:)';
40 l3=x(3,:)';
41 plot2d(V',[l1 l2 l3]);
42
43 xtitle('Figure E8-11.2', 'V', 'Fa,Fb,Fc' );
44 legend(['Fa';'Fb';'Fc']);

```

check Appendix [AP 19](#) for dependency:

8_12.sci

Scilab code Exa 8.12 clear

```
1 //clear//
2 clc
3 clear
4 exec("8.12data.sci");
5 t=1:10:250;
6 for i=1:length(t)
7 T(i)=2*t(i)+283;
8
9 k2(i)=4.58*exp((E2/1.987)*((1/500)-(1/T(i))))
10 k1(i)=3.3*exp((E1/1.987)*((1/300)-(1/T(i))))
11 Ca(i)=Cao/(1+tau*k1(i))
12 kappa=UA/(vo*Cao)/Cp
13 G(i)=-((tau*k1(i)/(1+k1(i)*tau))*DH1-(k1(i)*tau*k2(i)
      *tau*DH2/((1+tau*k1(i))*(1+tau*k2(i))));
14 Tc=(To+kappa*Ta)/(1+kappa);
15 Cb(i)=tau*k1(i)*Ca(i)/(1+k2(i)*tau);
16 R(i)=Cp*(1+kappa)*(T(i)-Tc);
17 Cc=Cao-Ca(i)-Cb(i);
18 F(i)=G(i)-R(i);
19 end
20 plot(T',[G R])
21
22 xtitle('Figure E8-12.1', 'T (K)', 'G(T),R(T)') ;
23 legend(['G(T)'; 'R(T)']);
```

Chapter 9

Unsteady State Nonisothermal Reactor Design

check Appendix [AP 14](#) for dependency:

9_1.sci

Scilab code Exa 9.1 clear

```
1 //clear//
2 clc
3 clear
4 exec("9.1 data . sci");
5 t = 0:10:1500;
6 function w=f(t,x)
7
8 w =zeros(1,1);
9
10 t1=535+90.45*x
11 k= .000273*exp(16306*((1/535)-(1/t1)));
12 w(1)=k*(1-x)
13 endfunction
14
15 X=ode([0],t0,t,f);
```

```

16 T=535+90.45*X;
17 scf(1)
18 plot2d(t,T);
19
20 xtitle( 'Figure E9-1.1', 't (Seconds)', 'T (oR)' ) ;
21
22 scf(2)
23 plot2d(t,X);
24
25 xtitle( 'Figure E9-1.1', 't (Seconds)', 'X' ) ;

```

check Appendix [AP 13](#) for dependency:

9_2.sci

Scilab code Exa 9.2 clear

```

1 //clear//
2 clc
3 clear
4 //this code is only for Part C
5 exec("9.2data.sci");
6 t = 55:1:121;
7 function w=f(t,Y)
8
9 w =zeros(2,1);
10
11
12
13 k=.00017*exp(11273/(1.987)*(1/461-1/Y(1)))
14 Qr=UA*(Y(1) -298)
15 Theata=Nbo/Nao
16 ra=-k*(Nao**2)*(1-Y(2))*(Theata-2*Y(2))/(U**2)
17 rate=-ra
18 Qg=ra*U*(dH)
19 w(1)=(Qg-Qr)/NCp

```

```

20 w(2)=(-ra)*U/Na0
21 endfunction
22
23 x=ode([467.992;0.0423],t0,t,f);
24
25
26 plot2d(t,x(1,:));
27
28 xtitle('Figure E9-2.2', 't', 'T (oC)') ;

```

check Appendix [AP 12](#) for dependency:

9_3.sci

Scilab code Exa 9.3 clear

```

1 //clear//
2 clc
3 clear
4 exec("9.3data.sci");
5 t = 0:1:360;
6
7 function w=f(t,Y)
8
9   w =zeros(5,1);
10
11 k=.39175*exp(5472.7*((1/273)-(1/Y(4))));
12 Cd=Y(3);
13
14 Kc=10^(3885.44/Y(4))
15 V=Vi+v0*t;
16 Fb0=Cb0*v0;
17 ra=-k*((Y(1)*Y(2))-((Y(3)*Cd)/Kc));
18 Na=V*Y(1)
19 Nb=V*Y(2)
20 Nc=V*Y(3)

```

```

21 rb=ra
22 rc=-ra
23 Nd=V*Cd
24 rate=-ra
25 NCp=cp*(Nb+Nc+Nd+Y(5))+cpa*Na;
26 w(1)=ra-(v0*Y(1))/V;
27 w(2) =rb+(v0*(Cb0-Y(2))/V);
28 w(3) =rc- (Y(3)*v0)/V;
29 w(4)= (UA*(Ta-Y(4))-Fb0*cp*(1+55)*(Y(4)-T0)+ra*V*dh)
      /NCp
30 w(5) =v0*Cw0
31 endfunction
32
33 x=ode([5;0.0001;00.0001;300;6.14],t0,t,f);
34 scf(1)
35 plot2d(t,x(4,:));
36
37 xtitle('Figure E9-3.1', 't', 'T' ) ;
38
39 scf(2)
40 l1=x(1,:)';
41 l2=x(2,:)';
42 l3=x(3,:)';
43 plot2d(t',[l1 l2 l3]);
44
45 xtitle('Figure E9-3.2', 't', 'Ca,Cb,Cc' ) ;
46 legend(['Ca';'Cb';'Cc']);

```

check Appendix [AP 11](#) for dependency:

9_4.sci

Scilab code Exa 9.4 clear

```

1 //clear//
2 clc

```



```

3 clear
4 //exec("9.3data.sci");
5 t = 0:.0001:4;
6 t0=0;
7 function w=f(t,Y)
8
9 w =zeros(5,1);
10
11 Fa0=80;
12 T0=75;
13 V=(1/7.484)*500;
14 UA=16000;
15 Ta1=60;
16 k=16.96e12*exp(-32400/1.987/(Y(5)+460));
17 Fb0=1000;
18 Fm0=100;
19 mc=1000;
20 ra=-k*Y(1);
21 rb=-k*Y(1);
22 rc=k*Y(1);
23 Nm=Y(4)*V;
24 Na=Y(1)*V;
25 Nb=Y(2)*V;
26 Nc=Y(3)*V;
27 ThetaCp=35+(Fb0/Fa0)*18+(Fm0/Fa0)*19.5;
28 v0=(Fa0/0.923)+(Fb0/3.45)+(Fm0/1.54);
29 Ta2=Y(5)-(Y(5)-Ta1)*exp(-UA/(18*mc));
30 Ca0=Fa0/v0
31 Cb0=Fb0/v0
32 Cm0=Fm0/v0
33 Q=mc*18*(Ta1-Ta2);
34 tau=V/v0;
35 NCp=Na*35+Nb*18+Nc*46+Nm*13.5;
36 w(1)=(1/tau)*(Ca0-Y(1))+ra;
37 w(2)=(1/tau)*(Cb0-Y(2))+rb;
38 w(3)=(1/tau)*(-Y(3))+rc;
39 w(4)=(1/tau)*(Cm0-Y(4));
40 w(5)=(Q-Fa0*ThetaCp*(Y(5)-T0)+(-36000)*ra*V)/NCp;

```

```

41 endfunction
42
43 x=ode([0;3.45;0;0;75],t0,t,f);
44 scf(1)
45 plot2d(t,x(1,:));
46
47 xtitle( 'Figure E9-4.1', 't', 'Ca' ) ;
48
49 scf(2)
50 plot2d(t,x(5,:));
51
52 xtitle( 'Figure E9-4.2', 't', 'T' ) ;
53 scf(3)
54 plot2d(x(5,:),x(1,:));
55
56 xtitle( 'Figure E9-4.3', 'T', 'Ca' ) ;

```

check Appendix [AP 10](#) for dependency:

9_8.sci

Scilab code Exa 9.8 clear

```

1 //clear//
2 clc
3 clear
4 exec("9.8data.sci");
5 t = 0:.01:1.5;
6
7 function w=f(t,Y)
8
9   w =zeros(4,1);
10
11 k1a=1.25*exp((9500/1.987)*((1/320)-(1/Y(4))));
12 k2b=0.08*exp((7000/1.987)*((1/290)-(1/Y(4))));
13 ra=-k1a*Y(1);

```

```

14 V=100+vo*t;
15 rc=3*k2b*Y(2);
16 rb=k1a*(Y(1)/2)-k2b*Y(2);
17 w(1)=ra+(Cao-Y(1))*vo/V;
18 w(2)=rb-Y(2)*vo/V;
19 w(3)=rc-Y(3)*vo/V; w(4)=(35000*(298-Y(4))-Cao*vo
    *30*(Y(4)-305)+((-6500)*(-k1a*Y(1))+(8000)*(-k2b*
    Y(2)))*V)/((Y(1)*30+Y(2)*60+Y(3)*20)*V+100*35);
20 endfunction
21
22 x=ode([1;0;0;290],t0,t,f);
23
24
25 scf(1)
26 l1=x(1,:)';
27 l2=x(2,:)';
28 l3=x(3,:)';
29 plot2d(t',[l1 l2 l3]);
30
31 xtitle('Figure E9-8.1', 't', 'Ca,Cb,Cc' );
32 legend(['Ca';'Cb';'Cc']);
33
34 scf(2)
35 plot2d(t,x(4,:));
36
37 xtitle('Figure E9-8.2', 't', 'T' );

```

Chapter 10

Catalysis and Catalytic Reactors

check Appendix [AP 9](#) for dependency:

10_3.sci

Scilab code Exa 10.3 clear

```
1 //clear//
2 clc
3 clear
4 exec("10.3data.sci");
5 w = 0:10:10000;
6
7 function W=f(w,x)
8
9     W=zeros(1,1);
10
11 pt0=.3*Po;
12 y=(1-alpha*w)^.5;
13 ph=pt0*(1.5-x)*y;
14 pt=pt0*(1-x)*y;
15 pb=2*pt0*x*y;
```

```

16 rt=-k*kt*ph*pt/(1+kb*pb+kt*pt);
17 rate=-rt;
18 W(1)=-rt/ft0;
19 endfunction
20 pt0=.3*Po;
21 X=ode([0],w0,w,f);
22
23
24 for i =1:length(X)
25     y(1,i)=(1-alpha*w(1,i))^.5;
26 ph(1,i)=pt0*(1.5-X(1,i))*y(1,i);
27 pt(1,i)=pt0*(1-X(1,i))*y(1,i);
28 pb(1,i)=2*pt0*X(1,i)*y(1,i)
29 end
30
31 m1 = X';
32 m2=y';
33 scf(1)
34 plot2d(w',[m1 m2]);
35
36 xtitle('Figure E10-3.1', 'w', 'x,y' );
37 legend(['x';'y']);
38
39 scf(2)
40 l1=ph'
41 l2=pt'
42 l3=pb'
43 plot2d(w',[l1 l2 l3]);
44
45 xtitle('Figure E10-3.2', 'w', 'ph,pt,pb' );
46 legend(['ph';'pt';'pb']);

```

check Appendix [AP 8](#) for dependency:

10_5.sci

Scilab code Exa 10.5 clear

```
1 //clear//
2 clc
3 clear
4 exec("10.5 data . sci");
5 t = 0:.01:.5;
6
7 function w=f(t,Y)
8
9     w =zeros(2,1);
10
11
12 ya0=Ca0/Ct0;
13 X=1-(1+ya0)/(1+Y(2)/Ct0)*Y(2)/Ca0;
14 w(1)=-kd*Y(1)*Y(2);
15 w(2) = (Ca0/tau)-((1+ya0)/(1+(Y(2)/Ct0))+tau*Y(1)*k)
        *Y(2)/tau;
16 endfunction
17
18 x=ode([1;.8],t0,t,f);
19 Ca0=.8;
20 Ct0=1
21 ya0=Ca0/Ct0;
22 for i=1:length(t)
23     X1(i)=1-(1+ya0)/(1+x(2,i)/Ct0)*x(2,i)/Ca0;
24     end
25
26
27 l1=x(1,: )'
28 l2=x(2,: )'
29 l3=X1;
30 plot2d(t',[l1 l2 l3]);
31
32 xtitle('Figure E10-5.1', 't', 'a,Ca,X' );
33 legend(['a';'Ca';'X']);
```

check Appendix [AP 7](#) for dependency:

10_7.sci

Scilab code Exa 10.7 clear

```
1 //clear//
2 clc
3 clear
4 exec("10.7data.sci");
5 z = 0:.1:10;
6 z0=0;
7 function w=f(z,X)
8
9     w =zeros(1,1);
10
11
12 U=Uo*(1+eps*X)
13 Pa=Pao*(1-X)/(1+eps*X)
14 Pb=Pao*X/(1+eps*X)
15 vo=Uo*3.1416*D*D/4
16 Ca0=Pao/R/T
17 Kca=Ka*R*T
18 Pc=Pb
19 a=1/(1+A*(z/U)**0.5)
20 raprime=a*(-kprime*Pa/(1+ Ka*Pa+Kb*Pb+Kc*Pc))
21 ra=rho*raprime;
22 w(1)=-ra/U/Ca0
23 endfunction
24
25 x=ode([0],z0,z,f);
26 for i=1:length(z)
27 U(1,i)=Uo*(1+eps*x(1,i))
28 a(1,i)=1/(1+A*(z(1,i)/U(1,i))**0.5)
29 end
30
31
```

```
32 l1=x(1,: )'  
33 l2=a(1,: )'  
34  
35 plot2d(z',[l1 l2]);  
36  
37 xtitle( 'Figure E10-7.1', 'z', 'X,a' ) ;  
38 legend(['X';'a']);
```

Scilab code Exa 13.8 clear

```
1 k=0.1  
2 cao=8;  
3 z0=0;
```

Chapter 11

External Diffusion Effects on Hetrogeneous Reactions

check Appendix [AP 6](#) for dependency:

11_1.sci

Scilab code Exa 11.1 clear

```
1 //clear//
2 clc
3 clear
4 exec("11.1data.sci");
5 WAZ1=DAB*CT0*(yAb-yAs)/s;
6 WAZ2=c*DAB*CT0*log((1-yAs)/(1-yAb))/s;
7 disp(WAZ1)
8 disp(WAZ2)
```

check Appendix [AP 5](#) for dependency:

11_3.sci

Scilab code Exa 11.3 clear

```
1 //clear//
2 clc
3 clear
4 exec("11.3data.sci");
5 //this is only Part A of the problem.
6 dp=(6*(D^2)*L/4)^(1/3);
7 disp("Particle diameter dp =")
8 disp(dp)
9 disp("m")
10 ac=6*(1-phi)*(1/dp);
11 disp("Surface area pervolume of bed =")
12 disp(ac)
13 disp("m^2/m^3")
14 Re =dp*U/v;
15 Y=(2*r*Lp+2*r^2)/dp^2;
16 Reprime=Re/((1-phi)*Y);
17 DAB=DAB0*(T/T0)^(1.75);
18 Sc=v/DAB;
19 Shprime=((Reprime)^.5)*Sc^(1/3);
20 kc=DAB*(1-phi)*Y*(Shprime)/(dp*phi);
21 X=1-exp(-kc*ac*z/U);
22 disp("X =")
23 disp(X)
```

check Appendix [AP 4](#) for dependency:

11_4.sci

Scilab code Exa 11.4 clear

```
1 //clear//
2 clc
3 clear
4 exec("11.4data.sci")
```

```
5 X2=1-(1/exp((log(1/(1-X1)))*(1/2)*((2)^.5)));
6 disp("X2 =")
7 disp(X2)
```

check Appendix [AP 3](#) for dependency:

11_5.sci

Scilab code Exa 11.5 clear

```
1 //clear//
2 clc
3 clear
4 exec("11.5 data.sci")
5 X2=1-(1/exp((log(1/(1-X1)))*((T2/T1)^(5/12))));
6 disp("X2 =")
7 disp(X2)
```

Chapter 13

Distributions of Residence Times for Chemical Reactions

check Appendix [AP 2](#) for dependency:

13_8.sci

Scilab code Exa 13.8 clear

```
1 //clear//
2 clc
3 clear
4 exec("13_8.sci");
5 z = 0:1:200;
6
7 function w=f(z,x)
8
9     w=zeros(1,1);
10
11 lam=200-z;
12 ca=cao*(1-x)
13 E1=4.44658e-10*(lam^4)-1.1802e-7*(lam^3)+1.35358e
    -5*(lam^2)-.00086
14 5652*lam+.028004;
```

```

15 E2=-2.64e-9*(lam^3)+1.3618e-6*(lam^2) -.00024069*lam
    +.015011
16 F1=4.44658e-10/5*(lam^5)-1.1802e-7/4*lam^4+1.35358e
    -5/3*lam^3-.000865652/2*lam^2+.028004*lam;
17 F2=-(-9.3076e-8*lam^3+5.02846e-5*lam^2-.00941*lam
    +.61823-1)
18 ra=-k*ca^2;
19 if lam< =70
20     E=E1
21 else
22     E=(E2)
23     end
24     if(lam< =70)
25         F=F1
26     else
27         F=F2
28     end
29     EF=E/(1-F)
30     w(1)=- (ra/cao+E/(1-F)*x)
31 endfunction
32
33 X=ode([0],z0,z,f);
34
35 plot2d(z,X);

```

check Appendix [AP 1](#) for dependency:

13_9.sci

Scilab code Exa 13.9 clear

```

1 //clear//
2 clc
3 clear
4 exec("13.9data.sci");
5 t = 0:.1:2.52;

```

```

6
7 function w=f(t,Y)
8
9 w=zeros(10,1);
10
11 E1=-2.104*t^4+4.167*t^3-1.596*t^2+0.353*t-.004
12 E2=-2.104*t^4+17.037*t^3-50.247*t^2+62.964*t-27.402
13 rc=k1*Y(1)*Y(2)
14 re=k3*Y(2)*Y(4)
15 ra=-k1*Y(1)*Y(2)-k2*Y(1)
16 rb=-k1*Y(1)*Y(2)-k3*Y(2)*Y(4)
17 if t<=1.26
18     E=E1
19 else
20     E=E2
21 end
22 rd=k2*Y(1)-k3*Y(2)*Y(4)
23
24 w(1)=ra
25 w(2)=rb
26 w(3)=rc
27 w(6)=Y(1)*E
28 w(7)=Y(2)*E
29 w(8)=Y(3)*E
30 w(4)=rd
31 w(5)=re
32 w(9)=Y(4)*E
33 w(10)=Y(5)*E
34 endfunction
35
36 X=ode([1;1;0;0;0;0;0;0;0;0],t0,t,f);
37
38 plot2d(t,X(1,:));

```

Chapter 14

Models for Nonideal Reactors

Scilab code Exa 14.3 clear

```
1 //clear//
2 clc
3 clear
4
5 t = 0:10:200;
6
7 function w=f(t,Y)
8
9     w =zeros(2,1);
10
11 CTe1=2000-59.6*t+.64*t^2-0.00146*t^3-1.047*10^(-5)*t
      ^4
12 Beta=.1
13 CTe2=921-17.3*t+.129*t^2-0.000438*t^3+5.6*10^(-7)*t
      ^4
14 alpha=.8
15 tau=40
16 if(t<80)
17     CTe=CTe1
18 else
19     CTe=CTe2
```

```

20 end
21
22 w(1)=(Beta*Y(2)-(1+Beta)*Y(1))/alpha/tau
23 w(2)=(Beta*Y(1)-Beta*Y(2))/(1-alpha)/tau
24 endfunction
25
26 X=ode([2000;0],t0,t,f);
27
28 t=t';
29 for i =1:length(t)
30 CTe1(i)=2000-59.6*t(i)+.64*(t(i)^2)-0.00146*(t(i)^3)
      -1.047*(10^(-5))*t(i)^4;
31 CTe2(i)=921-17.3*t(i)+.129*t(i)^2-0.000438*t(i)
      ^3+5.6*10^(-7)*t(i)^4
32 if(t(i)<80)
33     CTe(i)=CTe1(i)
34 else
35     CTe(i)=CTe2(i)
36 end
37 end
38
39
40 l1=X(1,: )';
41 l2=CTe;
42
43 plot2d(t,[l1 l2]);
44
45 xtitle('Figure E14-3.1', 't', 'CT1,CTe' );
46 legend(['CT1';'CTe']);

```

Appendix

Scilab code AP 1 data

```
1 k1=1;  
2 k2=1;  
3 k3=1;  
4 t0=0;
```

Scilab code AP 2 data

```
1 k=0.1  
2 cao=8;  
3 z0=0;
```

Scilab code AP 3 data

```
1 X1=.865;  
2 T1=673;  
3 T2=773;
```

Scilab code AP 4 data

```
1 X1=.865;
```

Scilab code AP 5 data

```
1 D=.0025; //m  
2 L=.005; //m  
3 phi=.3;
```

```
4 U=15; //m/s;
5 v=4.5e-4; //m^2/s
6 r=.0025/2;
7 Lp=.005;
8 DAB0=.69e-4;
9 T=750;
10 T0=298;
11 z=.05; //m
```

Scilab code AP 6 data

```
1 DAB =1e-6;
2 CT0=.1; //kmol/m^3
3 yAb=.9;
4 yAs=.2;
5 s=1e-6;
6 c=.1;
```

Scilab code AP 7 data

```
1 Ka=0.05;
2 Kb=.15;
3 Pao=12;
4 eps=1;
5 A=7.6;
6 R=0.082;
7 T=400+273;
8 Kc=.1;
9 rho=80;
10 kprime=0.0014;
11 D=1.5;
12 Uo=2.5;
```

Scilab code AP 8 data

```
1 kd=9;
2 Ca0=.8;
```

```
3 tau=.02
4 k=45;
5 Ct0=1;
6 t0=0
```

Scilab code AP 9 data

```
1 ft0=50
2 k=.0000000145*1000*60;
3 kt=1.038;
4 kb=1.39;
5 alpha=0.000098;
6 Po=40;
7 w0=0;
```

Scilab code AP 10 data

```
1 Cao=4;
2 vo=240;
3 t0=0;
```

Scilab code AP 11 data

```
1 Fa0=80;
2 T0=75;
3 V=(1/7.484)*500;
4 UA=16000;
5 Ta1=60;
6 Fb0=1000;
7 Fm0=100;
8 mc=1000;
9 t0=0;
```

Scilab code AP 12 data

```
1 v0=.004;
2 Cb0=1;
```

```
3 UA=3000;  
4 Ta=290;  
5 cp=75240;  
6 T0=300;  
7 dh=-7.9076e7;  
8 Cw0=55;  
9 cpa=170700;  
10 Vi=.2;  
11 t0=0;
```

Scilab code AP 13 data

```
1 NCp=2504;  
2 U=3.265+1.854i;  
3 Nao=9.0448;  
4 UA=35.83;  
5 dH=-590000;  
6 Nbo=33;  
7 t0=55;
```

Scilab code AP 14 data

```
1 t0=0;
```

Scilab code AP 15 data

```
1 T = [300:10:600]';
```

Scilab code AP 16 data

```
1 Fa0 = .9*163;  
2 Ca0 = 9.3;  
3 V0 = 0;
```

Scilab code AP 17 data

```
1 T =[535 550 565 575 585 595 605 615 625]';
```

```
2 HOC= -226000;
3 HOB = -123000;
4 HOA = -66600;
5 CpC = 46;
6 CpB = 18;
7 CpA = 35;
8 CpM = 19.5;
9 TR = 528;
10 Ti0 = 535;
11 vA0 = 46.62;
12 vB0 = 46.62;
13 VM0 = 233.1;
14 V = 40.1;
15 FA0 =43.04;
16 FM0 = 71.87;;
17 FB0 = 802.8;
18 A = 16.96e12;
19 E = 32400;
20 R = 1.987;
```

Scilab code AP 18 data

```
1 HONH3 = -11020; // cal/moleN2
2 HOH2 = 0;
3 HN2 = 0;
4 CpNH3 = 8.92; // cal/moleH2.K
5 CpH2 = 6.992; // cal/moleN2.K
6 CpN2 =6.984; // cal/moleNH3.K
7 T = 423; //K
8 TR = 298; //K
```

Scilab code AP 19 data

```
1 Cp=200
2 Cao=0.3
3 To=283
4 tau=.01;
5 DH1=-55000;
```

```
6 DH2=-71500;
7 vo=1000;
8 E2=27000;
9 E1=9900;
10 UA=40000;
11 Ta=330;
```

Scilab code AP 20 data

```
1 V0=0;
2 Cto=0.1;
3 To=423;
```

Scilab code AP 21 data

```
1 ysc=1/.08;
2 ypc = 5.6;
3 ks = 1.7;
4 m = 0.03;
5 umax = .33;
6 t0 = 0;
```

Scilab code AP 22 data

```
1 Km = 0.0266;
2 Vmax1 = 1.33;
3 Et2 = 0.001;
4 Et1 = 5;
5 X = .8;
6 Curea0 = .1;
```

Scilab code AP 23 data

```
1 Curea = [.2 .02 .01 .005 .002]';
2 rurea = -[1.08 .55 .38 .2 .09]';
```

Scilab code AP 24 data

```
1 v0 =0;
```

Scilab code AP 25 data

```
1 k1= 55.2;  
2 k2=30.2;  
3 t0=0;
```

Scilab code AP 26 data

```
1 CCH4 = [2.44 4.44 10 1.65 2.47 1.75] '*1e-4;  
2 PC0= [1 1.8 4.08 1 1 1]';  
3 v0 =300;  
4 W= 10;
```

Scilab code AP 27 data

```
1 CCH4 = [2.44 4.44 10 1.65 2.47 1.75] '*1e-4;  
2 PC0= [1 1.8 4.08 1 1 1]';  
3 v0 =300;  
4 W= 10;
```

Scilab code AP 28 data

```
1 CHCl= [1 4 2 .1 .5];  
2 rHCl = [1.2 2 1.36 .36 .74]*1e7;
```

Scilab code AP 29 data

```
1 t = [0 2.5 5 10 15 20]';  
2 P = [7.5 10.5 12.5 15.8 17.9 19.4]';  
3 P0 = 7.5;
```

Scilab code AP 30 data

```
1 ka = 2.7;  
2 kc = 1.2;
```

```
3 Ct0 = .1;
4 fa0 =10;
5 V0 = 0;
```

Scilab code AP 31 data

```
1 FA0 = 440;
2 P0 = 2000;
3 Ca0 = .32;
4 R = 30;
5 phi = .4;
6 kprime = 0.02; //lb.mol/atm.lb cat.h
7 L = 27;
8 rhocat = 2.6;
9 m=44;
10
11 alpha = 0.0166;
12 e = -0.15;
13 Z0 = 0;
```

Scilab code AP 32 data

```
1 kprime = 0.0266; //lb.mol/atm.lb cat.h
2 alpha = 0.0166;
3 e = -0.15;
4 W0 = 0;
5 FA0=1;
```

Scilab code AP 33 data

```
1 k = 0.0141; //lb.mol/atm.lb cat.h
2 FA0 = 1.08; //lb.mol/h
3 FBO = 0.54; // lb.mol/h
4 FI = 2.03; // lb.mol/h
5 bita0 = 0.0775; // atm/ft
6 Ac = 0.01414; // ft^2
7 phi = 0.45;
```



```
8 rhoc = 120; // lb cat/ft^3
9 P0 = 10; // atm
10 X = 0.6;
```

Scilab code AP 34 data

```
1 Ac = 0.01414; // ft^2
2 m = 104.4; // lbm/h
3 mu = 0.0673; // lbm/ft.h
4 Dp = 0.0208; // ft
5 gc = 4.17e8; // lbm.ft/lbf.h^2
6 phi = 0.45;
7 rho = 0.413; // lbm/ft^3
8 P0 = 10; // atm
9 L = 60; // ft
```

Scilab code AP 35 data

```
1 k1 = 0.072; // s^-1;
2 yA0 = 1;
3 P0= 6; //atm
4 R = 0.73; // atm/lb.mol.oR
5 T0 = 1980; //oR
6 T1 = 1000; //K
7 T2 = 1100; // K
8 e=1;
9 E = 82000; // cal/g.mol
10 FB= 0.34; //lb.mol/s
11 X = 0.8;
```

Scilab code AP 36 data

```
1 k = 0.311; // min^-1;
2 FC= 6.137; //lb.mol/min
3 X = 0.8;
4 CA01= 1; //mol/dm^3
```

Scilab code AP 37 data

```
1 k= 2.2;
2 v00 = .05;
3 Cb0 = .025;
4 v0 = 5;
5 Ca0 = .05;
6 t0 = 0;
```

Scilab code AP 38 data

```
1 kc = 0.2;
2 Ct0 = .2;
3 k = .7;
4 V0= 0;
```

Scilab code AP 39 data

```
1 t = [0 0.5 1 1.5 2 3 4 6 10];
2 CC = [0 0.145 .27 .376 .467 .61 .715 .848 .957];
3 CA0 = 1;
```

Scilab code AP 40 data

```
1 CA0 = 10;
2 CB0 = 2;
3 X = 0.2;
4 X1=0.9
```

Scilab code AP 41 data

```
1 FA0 = 0.867; // mol/s
2 X1 = 0.5;
3 X2 = 0.8;
4 rA2 = -(1/800);
5 X = [0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8]';
6 p = [189 192 200 222 250 303 400 556 800]; //1/-rA =
      800//dm^3.s/mols
```

Scilab code AP 42 data

```
1
2 clc
3 clear
4 exec(" 2.6 data . sci");
5
6
7 X1 = X(1:5);
8 p1 = p(1:5);
9 V1 = FA0*inttrap(X1,p1)
10 X2 = X(5:9);
11 p2 = p(5:9);
12 V2 = FA0*inttrap(X2,p2)
13 V=V1+V2;
14 disp("V1 =")
15 disp(V1)
16 disp("dm^3")
17 disp("V2 =")
18 disp(V2)
19 disp ("dm^3")
20 disp("V =")
21 disp(V)
22 disp ("dm^3")
```

Scilab code AP 43 data

```
1 FA0 = 0.867; // mol/s
2 rA = -(1/250);
3 rA2 = -(1/800);
4 X = 0.8;
5 X1 = 0.4;
6 X2 = 0.8
```

Scilab code AP 44 data

```
1 FA0 = 5; // mol/s
2 rAat=-(1/400);
```

```
3
4 X = [0 0.1 0.2 0.3 0.4 0.5 0.6]';
5 p = [189 192 200 222 250 303 400]; //1/-rA = 800//dm
    ^3.s/mols
```

Scilab code AP 45 data

```
1 P0 = 10; //atm
2 yA0 = 0.5;
3 T0 = 422.2; //K
4 R = 0.082; // dm^3.atm/mol.K
5 v0 = 6; //dm^3/s
6 X = [0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8]';
7 p = [189 192 200 222 250 303 400 556 800]; //1/-rA =
    800//dm^3.s/mols
```

Scilab code AP 46 data

```
1 P0 = 10; //atm
2 yA0 = 0.5;
3 T0 = 422.2; //K
4 R = 0.082; // dm^3.atm/mol.K
5 v0 = 6; //dm^3/s
6 X = 0.8;
7 rA = -1/800; //1/-rA = 800//dm^3.s/mol
```

Scilab code AP 47 data

```
1 P0 = 10; //atm
2 yA0 = 0.5;
3 T0 = 422.2; //K
4 R = 0.082; // dm^3.atm/mol.K
5 v0 = 6; //dm^3/s
```
