Scilab Textbook Companion for
Elements Of Chemical Reaction Engineering
by H. S. Fogler[1]

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Book Description

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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.

Contents

List of Scilab Codes

Chapter 1

Mole Balances

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

Scilab code Exa 2.1 clear

```
1  // clear //
2  clc
3  clear
4  exec("2.1data.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")
```

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 ")
```

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 differennt from the book
       because inttrap command of SCILAB uses
       trapezoidal integration , while in book it has
       been calculated using five point formulae . ")
```

Scilab code Exa 2.4 clear

```
1  // clear //
2  clc
3  clear
4  exec("2.4 data.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")
```

Scilab code Exa 2.5 clear

```
1  // clear //
2  clc
3  clear
4  exec("2.5 data.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")
```

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")
```

Scilab code Exa 2.7 clear

```
 1  //clear//
 2  clc
 3  clear
 4  exec("2.7 data.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

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/dm^3")
20 disp("CB =")
21 disp(CB1)
```

```
22   disp("mol/dm^3")
```

Chapter 4

Isothermal Reactor Design

Scilab code Exa 4.1 clear

```
1  //clear//
2  clc
3  clear
4  exec("4.1data.sci");
5
6  x=t;
7  y =((CA0-CC)/CA0);
8
9  yi=interpln([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")
```

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)
```

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")
```

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))^.5)*P0;
10 deltaP = P0 - P;
11
12 disp("deltaP")
13 disp(deltaP)
14 disp("atm")
```

Scilab code Exa 4.6 clear

```scilab
1  //clear//
2  clc
3  clear
4  exec("4.6data.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")
```

Scilab code Exa 4.7 clear

```scilab
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  end
22  rate =rate';
23
24  scf(1)
25  plot2d(W,rate);
26  xtitle( 'Figure E4-7.1 Reaction rate porfile down
      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']);
```

Scilab code Exa 4.8 clear

```
1  // clear //
2  clc
3  clear
4  exec("4.8data.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']);
```

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']);
```

Scilab code Exa 4.10 clear

```
1  //clear//
2  clc
3  clear
4  exec("4.10data.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']);
```

Scilab code Exa 4.11 clear

```
1   //clear//
2   clc
3   clear
4   exec("4.11data.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
```

Scilab code Exa 5.2 Clear

```
1 //clear//
2 clc
3 clear
4 exec("5.2data.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' ) ;
```

Scilab code Exa 5.3 Clear

```
1  //Clear//
2  clc
3  clear
4  exec("5.3data.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)' ) ;
```

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

Scilab code Exa 6.6 Clear

```
1  // Clear //
2  clc
3  clear
4  exec("6.6 data.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']);
```

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;
```

27

```
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

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)
```

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")
```

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);
```

30

```
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

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")
```

Scilab code Exa 8.4 clear

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

```
3  clear
4  exec("8.4 data.sci");
5  HRx0 = H0C-H0B-H0A;
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']);
```

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)
        *360)));
25
26    ra(1,i) = k(1,i)*Ca0*(1-(1+(1/Kc(1,i)))*x(1,i));
27  end
28  scf(1)
29  plot2d(V,x(1,:));
30
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
        )' ) ;
```

Scilab code Exa 8.7 clear

```
1  //clear//
2  clc
3  clear
4  //this code is only for the first part of the
      problem (Adiabatic PFR)
5  exec("8.7data.sci");
6   V = 0:.1:5;
7  function w=f(V,Y)
8
9   w =zeros(2,1);
10
11 k=(8.2e14)*exp(-34222/Y(1));
12
13 Cpa = 26.63+.183*Y(1)-(45.86e-6)*(Y(1)^2);
14 delCp = 6.8-(11.5e-3)*Y(1)-(3.81e-6)*(Y(1)^2);
15 deltaH = 80770+6.8*(Y(1)-Tr)-(5.75e-3)*((Y(1)^2)-Tr
      ^2)-(1.27e-6)*((Y(1)^3)-Tr^3);
16 ra = -k*Ca0*(((1-Y(2))/(1+Y(2)))*(T0/Y(1)));
17 w(1) = -ra*(-deltaH)/(Fa0*(Cpa+Y(2)*delCp));
18 w(2)= -ra/Fa0;
19
20 endfunction
21
22 x=ode([1035;0],V0,V,f);
23 scf(1)
24 plot2d(V,x(1,:));
25
26 xtitle( 'Figure E8-7.1', 'V (m^3)', 'T (K)' ) ;
27
28 scf(2)
29 plot2d(V,x(2,:));
30
```

```
31  xtitle( 'Figure E8-7.1', 'V (m^3)', 'X' ) ;
```

Scilab code Exa 8.8 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+
           100000*exp(-33.78*(T(i)-298)/T(i)));
7     XEB(i) = (2.5e-3)*(T(i)-300);
8  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)/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,:));
```

Scilab code Exa 8.10 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)/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,:));
```

Scilab code Exa 8.11 clear

```
1 //clear//
2 clc
3 clear
4 exec("8.11data.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']);
```

Scilab code Exa 8.12 clear

```
1  //clear//
2  clc
3  clear
4  exec("8.12 data.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

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' );
```

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/Nao
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)' ) ;
```

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
```

44

```
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']);
```

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' ) ;
```

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 1 for dependency:

```
10_3.sci
```

Scilab code Exa 10.3 clear

```
1  // clear //
2  clc
3  clear
4  exec("10.3 data.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']);
```

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']);
```

Scilab code Exa 1.7 clear

```
1  //clear//
2  clc
3  clear
4  //exec("9.8data.sci");
5  t = 0:.01:.5;
6
7  function w=f(t,Y)
8
9   w =zeros(2,1);
10
11  d(X)/d(z}=-ra/U/Ca0
12  Ka=0.05;
13  Kb=.15;
14  Pao=12;
15  eps=1;
16  A=7.6;
17  R=0.082;
18  T=400+273;
19  Kc=.1;
20  rho=80;
21  kprime=0.0014;
22  D=1.5;
23  Uo=2.5
24  U:Uo*(1+eps*X)
25  Pa=PBo*(1-X)/(1tepstX)
26  Pb=Pao*X/(1+eps*X)
27  vo=Uo*3.1416*D*D/4
28  Ca0=PBo/R/T
29  Kca=Ka*R*T
30  Pc=Pb
31  a=1/(1+At(z/U)**0.S)
32  raprime=at (-kprirne*Pa/(1 t Kat Pa+Kb:1:Pb+Kct  P c
33  ra:rhotraprime
34  endfunction
35
36  x=ode([1;.8],t0,t,f);
37  Ca0=.8;
38  Ct0=1
```

```
39 ya0 = Ca0 / Ct0 ;
40 for i =1: length ( t )
41    X ( i ) =1 -(1+ ya0 ) /(1+ x (2 , i ) / Ct0 )* x (2 , i ) / Ca0 ;
42    end
43 plot2d ( t , x (1 ,:) ) ;
44
45 plot2d ( t , x (2 ,:) ) ;
46 plot2d ( t , X ) ;
```

Scilab code Exa 10.7 clear

```
1  // clear //
2  clc
3  clear
4  exec ( " 10.7 data . 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
```

53

```
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']);
```

Chapter 11

External Diffusion Effects on Hetrogeneous Reactions

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)
```

Scilab code Exa 11.3 clear

```
1 clc
2 clear
3 exec("11.3data.sci");
4 //this is only Part A of the problem.
5 dp=(6*(D^2)*L/4)^(1/3);
```

```
 6 disp("Particle diameter dp =")
 7 disp(dp)
 8 disp("m")
 9 ac=6*(1-phi)*(1/dp);
10 disp("Surface area pervolume of bed =")
11 disp(ac)
12 disp("m^2/m^3")
13 Re =dp*U/v;
14 Y=(2*r*Lp+2*r^2)/dp^2;
15 Reprime=Re/((1-phi)*Y);
16 DAB=DAB0*(T/T0)^(1.75);
17 Sc=v/DAB;
18 Shprime=((Reprime)^.5)*Sc^(1/3);
19 kc=DAB*(1-phi)*Y*(Shprime)/(dp*phi);
20 X=1-exp(-kc*ac*z/U);
21 disp("X =")
22 disp(X)
```

Scilab code Exa 11.4 clear

```
1 clc
2 clear
3 exec("11.4data.sci")
4 X2=1-(1/exp((log(1/(1-X1)))*(1/2)*((2)^.5)));
5 disp("X2 =")
6 disp(X2)
```

Scilab code Exa 11.5 clear

```
1 //clear//
2 clc
3 clear
4 exec("11.5data.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

Scilab code Exa 13.8 clear

```
1  //clear//
2  clc
3  clear
4  exec("13.8data.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);
```

Scilab code Exa 13.9 clear

```
1  clc
2  clear
3  exec("13.9 data.sci");
4  t = 0:.1:2.52;
5
6  function w=f(t,Y)
7
8    w =zeros(10,1);
9
10  E1=-2.104*t^4+4.167*t^3-1.596*t^2+0.353*t-.004
11  E2=-2.104*t^4+17.037*t^3-50.247*t^2+62.964*t-27.402
12  rc=k1*Y(1)*Y(2)
```

```
13  re=k3*Y(2)*Y(4)
14  ra=-k1*Y(1)*Y(2)-k2*Y(1)
15  rb=-k1*Y(1)*Y(2)-k3*Y(2)*Y(4)
16  if t< =1.26
17    E=E1
18  else
19    E=E2
20    end
21    rd=k2*Y(1)-k3*Y(2)*Y(4)
22
23    w(1)=ra
24  w(2) =rb
25  w(3) =rc
26  w(6)=Y(1)*E
27  w(7)=Y(2)*E
28  w(8)=Y(3)*E
29  w(4)=rd
30  w(5) =re
31  w(9)=Y(4)*E
32  w(10)=Y(5)*E
33  endfunction
34
35  X=ode([1;1;0;0;0;0;0;0;0;0],t0,t,f);
36
37  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  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;
```