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

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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.

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Mole Balances

Scilab code Exa 1.3 Find V

```
1 // clear //
2 clc
3 clear
4 exec("1.3 data.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")
```

Conversion and Reactor Sizing

Scilab code Exa 2.1 calculate mole

```
1 //clear//
2 clc
3 clear
4 exec("2.1data.sci");
5 CAO=(yAO*PO)/(R*TO);
6 FAO = CAO*vO;
7 disp("CAO =")
8 disp(CAO)
9 disp ("mol/dm^3")
10 disp(FAO =")
11 disp(FAO)
12 disp("mol/s")
```

Scilab code Exa 2.2 Volume

```
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 Volume

```
1 //clear//
2 clc
3 clear
4 exec("2.3 data.sci");
5 CAO = (yAO * PO) / (R * TO);
6 \text{ FAO} = \text{CAO} * \text{vO};
7 /V = FA0*X*(1/-rA)
9 V = FA0*inttrap(X,p)
10 disp("FA0 =")
11 disp(FAO)
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.")
```

Scilab code Exa 2.4 clear

```
1 //clear//
2 clc
3 clear
4 exec("2.4data.sci");
5
6
7 VCSTR = FAO*X(7)*(1/-rAat);
8 VPFR = FAO*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 = FAO*X1*(1/-rA);
8 V2 = FAO*(X2-X1)*(1/-rA2);
9 V = FAO*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 // \operatorname{clear} //
2 clc
3 clear all
4 exec("2.6 data.sci");
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 \text{ disp}("V =")
21 disp(V)
22 disp ("dm<sup>3</sup>")
```

Scilab code Exa 2.7 clear

```
1 // clear //
2 clc
3 clear
4 exec("2.7data.sci");
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 \text{ disp}("V1 =")
13 disp(V1)
14 disp("dm^3")
15 \text{ disp}("V2 =")
16 disp(V2)
17 disp ("dm^3")
18 disp("V =")
19 disp(V)
20 disp ("dm^3")
```

Rate Laws and Stoichiometry

Scilab code Exa 3.5 clear

```
1 // \operatorname{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 \text{ 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<sup>3</sup>")
20 disp("CB =")
21 disp(CB1)
```

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 =((CAO-CC)/CAO);
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");
6
   FAO = FC/X;
    vAO = FAO/CAO1;
    vBO = vAO;
8
9
    v0 = vAO + vBO;
10
    V = v0*X/(k*(1-X));
11
12
    // CSTR in parallel
13
    V1 = 800/7.48;
14
    Tau = V1/(v0/2);
15
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("4.5 data.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

```
1 // clear //
2 clc
3 clear
4 exec("4.6 data.sci");
6 	ext{ FTO} = 	ext{FAO+FBO+FI};
7 \text{ yAO} = \text{FAO/FTO};
8 e = yA0*(1-.5-1);
9 \text{ PAO} = yA0*PO;
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

```
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
     F(i) = (1+e*x(1,i))/x(2,i);
17 \text{ end}
18 F= F;
19 for i = 1:61
     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 \quad 11 = x(1, :)
30 \ 12=x(2,:)
31 \quad 13 = F'
32 plot2d(W',[11 12 13]);
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);
```

```
Ca = Ca0*(1-Y(1))*Y(2)/(1+Y(1));
10
11
   ra =kprime*Ca*rhocat*(1-phi);
12
   G = m/Ac;
   V = 3.14*(Z*(R^2) - (1.3*(Z-L)^3) - (1/3)*L^3)
13
14 bita = (98.87*G+25630*G^2)*0.01;
15 W=rhocat*(1-phi)*V
16 \text{ w(1)} = -\text{ra*Ac/FAO}
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)
     V(1,i) = 3.14*Z(1,i)*((R^2)-(Z(1,i)-L)^2)
23
      W1(1,i) = rhocat*(1-phi)*V(1,i)
24
25 end
26
27 \quad 11=x(1,:)
28 \quad 12 = x(2, :)
29
30 plot2d(W1',[11 12]);
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("4.9 data.sci");
5 V = 0:1:100;
6 function w=f(V,fa)
7
8 w=zeros(1,1);
```

```
ft = 2*(fa0-fa(1))
10 Ca = Ct0*fa(1)/ft;
    fb = 2*(fa0-fa(1));
11
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 \text{ for } i = 1:101
      fb(1,i) = 2*(fa0-x(1,i));
21
22 \text{ end}
23 \quad 11 = x';
24 12=fb';
25
26 plot2d(V',[11 12]);
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("4.10 data.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 \quad 11 = x(1, :)
22 	12=x(2,:)
23 \quad 13=x(3,:)
24 plot2d(V',[11 12 13]);
25
26 xtitle ('Figure E4-10.2', 'V', 'Fa, Fb, Fc');
27 legend(['Fa'; 'Fb'; 'Fc']);
```

Scilab code Exa 4.11 clear

```
1 // \operatorname{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;
   w(1) = -k*C(1)*C(2)-v00*C(1)/v;
11
   w(2) = -k*C(1)*C(2)+v00*(Cb0-C(2))/v;
12
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 \ 11=x(1,:)
21 \quad 12=x(2,:)
22 \quad 13=x(3,:)
23 for i = 1:length(t)
     rate(1,i)=k*x(1,i)*x(2,i)
25
     end
26 scf(1)
27 plot2d(t',[11 12 13]);
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
```

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("5.2 data.sci");
5 for i =1:length(t)
6 g(i) =log(2*P0/(3*P0-P(i)));
```

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)');
```

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)

Multiple Reactions

Scilab code Exa 6.6 Clear

```
1 // Clear //
2 clc
3 clear
4 exec("6.6 data.sci");
5 \quad t = 0:.01:.5;
6 function w=f(t,c)
8
   w = zeros(3,1);
10 r1 = -k1*c(2)*c(1)^.5;
11 r2 = -k2*c(3)*c(1)^.5;
12 \quad w(1) = r1 + r2;
13 \quad w(2) = r1;
14
   w(3) = -r1+r2;
15
16 endfunction
17
18 x = ode([.021;.0105;0],t0,t,f);
19
20 \ 11=x(1,:)
21 \quad 12=x(2,:)
```

```
22 13=x(3,: )'
23
24 plot2d(t',[11 12 13]);
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 // \operatorname{clear} //
2 clc
3 clear
4 exec("6.8 data.sci");
   v = 0:.1:10;
6 function w =FF(v,f)
7
8
    w = zeros(6,1);
    ft = f(1)+f(2)+f(2)+f(4)+f(5)+f(6);
    r1a = -5*8*(f(1)/ft)*(f(2)/ft)^2;
10
11
    r2a = -2*4*(f(1)/ft)*(f(2)/ft);
12
    r4c = -5*3.175*(f(3)/ft)*(f(1)/ft)^(2/3);
    r3b = -10*8*((f(3)/ft)^2)*(f(2)/ft);
13
14
   Ca = 2*f(1)/ft;
    Cb = 2*f(2)/ft;
15
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 \text{ 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],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']);
```

Nonelementary Reaction Kinetics

Scilab code Exa 7.7 clear

```
1 // \operatorname{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));
    slope = (y(5)-y(1))/(x(5)-x(1));
    plot2d(x,y)
10
11
    xtitle('Figure E7-7.1', '1/Curea', '1/-rurea');
12
13
    disp("(Km/Vma = slope")
14
    disp(slope)
15
```

Scilab code Exa 7.8 clear

```
1 // clear //
2 clc
3 clear
4 exec("7.8 data.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("7.9 data.sci");
5 t = 0:.1:12;
6 function w=f(t,c)
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;
   w(2) = ysc*(-rg)-rsm;
16
   w(3) = rg*ypc;
17
18
19 endfunction
20
21 x = ode([1;250;0],t0,t,f);
```

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*HONH3-3*HOH2-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 \text{ HRxO} = \text{HOC-HOB-HOA};
6 deltaCp = CpC-CpB-CpA;
7 deltaHRx0 = HRx0+deltaCp*(TR-TR);
8 \quad vO = vAO + vBO + VMO;
9 tau = V/v0;
10 CAO = FAO/vO;
11 \text{ phiMO} = \text{FMO/FAO};
12 \text{ phiBO} = FBO/FAO;
13 Cpi = CpA+phiB0*CpB+phiM0*CpM;
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))))
      (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
  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 \quad 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 \text{ end}
28 scf(1)
29 plot2d(V,x(1,:));
30
31 xtitle ('Figure E8-6.1a', 'V(m^3)', 'X');
32 \text{ 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 // \operatorname{clear} //
2 clc
3 clear
4 //this code is only for the first part of the
      problem (Adiabatic PFR)
5 exec("8.7 data.sci");
   V = 0:.1:5;
7 function w=f(V,Y)
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 \text{ 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

Scilab code Exa 8.9 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 \text{ 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 \text{ Pao} = .22
21 thetao=.91
22 \text{ eps} = -.055
23 R = 1.987;
24 Kp = exp(42311/R/Y(3)-11.24);
25 \text{ 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 \, \text{end}
31
32 \text{ w}(1) = (-1.12*10**(-8)*(1-.055*Y(2))*Y(3))*(5500*visc
       +2288)/Y(1);
33 \text{ w}(2) = -(\text{ra})/\text{fao};
34 \text{ w}(3) = (5.11*(Ta-Y(3))+(-ra)*(-deltah))/(fao*(summ+Y)
       (2)*dcp))
35 endfunction
36
37 \text{ X} = \text{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 \text{ WO=0};
7 function w=f(W,Y)
     w = zeros(3,1);
9
10
11 \text{ fao} = .188
12 \text{ visc} = .090
13 \text{ 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 \text{ Po} = 2
20 \text{ Pao} = .22
21 thetao=.91
22 \text{ eps} = -.055
23 R=1.987;
24 Kp = exp(42311/R/Y(3)-11.24);
25 \text{ if}(Y(2) < =.05)
26
27
     ra=(-k*(.848-.012/(Kp**2)));
28 else
     ra=(-k*(1-Y(2))/(thetaso+Y(2)))**.5*(Y(1)/Po*Pao
29
         *((thetao - .5*Y(2))/((1+eps*Y(2)))-((thetaso+Y))
         (2))/(1-Y(2)))**2/(Kp**2));
30 end
31
32 \text{ w}(1) = (-1.12*10**(-8)*(1-.055*Y(2))*Y(3))*(5500*visc
      +2288)/Y(1);
33 \text{ w}(2) = -(\text{ra})/\text{fao};
34 \text{ 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("8.11 data.sci");
5 V = 0:.01:1;
7 function w=f(V,Y)
    w = zeros(4,1);
9
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 \text{ w}(2) = -r1a;
24
25 \text{ w}(3) = -r2a/2;
```

```
26 \text{ w}(4) = (4000*(373-Y(4))+(-r1a)*20000+(-r2a)*60000)
      /(90*Y(1)+90*Y(2)+180*Y(3));
27 endfunction
28
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 \ 11=x(1,:)
39 12=x(2,:)
40 \quad 13=x(3,:)
41 plot2d(V',[11 12 13]);
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
```

Unsteady State Nonisothermal Reactor Design

Scilab code Exa 9.1 clear

```
1 // \operatorname{clear} //
2 clc
3 clear
4 exec("9.1 data.sci");
5 t = 0:10:1500;
6 function w=f(t,x)
8
   w = zeros(1,1);
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 \quad T = 535 + 90.45 * X;
17 scf(1)
18 plot2d(t,T);
```

```
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("9.2 data.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 // \operatorname{clear} //
2 clc
3 clear
4 exec("9.3 data.sci");
5 t = 0:1:360;
7 function w=f(t,Y)
9 \quad 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 \text{ rb=ra}
22 \text{ rc=-ra}
23 \text{ Nd} = \text{V} * \text{Cd}
24 rate=-ra
NCp = cp*(Nb+Nc+Nd+Y(5))+cpa*Na;
26 \text{ w(1)} = \text{ra} - (\text{v0} * \text{Y(1)}) / \text{V};
27 \text{ w}(2) = \text{rb} + (\text{v0} * (\text{Cb0} - \text{Y}(2)) / \text{V});
28 \text{ w(3)} = \text{rc-} (Y(3)*v0)/V;
29 w(4) = (UA*(Ta-Y(4))-Fb0*cp*(1+55)*(Y(4)-T0)+ra*V*dh)
        /NCp
```

```
30 \text{ w (5)} = \text{v0} * \text{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 \quad 11=x(1,:)
41 12=x(2,:),
42 \ 13=x(3,:)
43 plot2d(t',[11 12 13]);
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("9.3 data.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 \text{ ra}=-k*Y(1);
21 \text{ rb=-k*Y(1)};
22 \text{ rc=k*Y(1)};
23 Nm = Y(4) * V;
24 \text{ Na=Y}(1)*V;
25 \text{ Nb=Y}(2)*V;
26 \text{ Nc} = Y(3) * V;
27 ThetaCp=35+(Fb0/Fa0)*18+(Fm0/Fa0)*19.5;
v0 = (Fa0/0.923) + (Fb0/3.45) + (Fm0/1.54);
29 Ta2=Y(5)-(Y(5)-Ta1)*exp(-UA/(18*mc));
30 \text{ CaO} = \text{FaO}/\text{vO}
31 \text{ CbO} = \text{FbO/vO}
32 \quad CmO = FmO / vO
33 Q=mc*18*(Ta1-Ta2);
34 \text{ tau=V/v0};
35 NCp=Na*35+Nb*18+Nc*46+Nm*13.5;
36 \text{ w}(1) = (1/\text{tau}) * (\text{Ca}0 - \text{Y}(1)) + \text{ra};
37 \text{ w}(2) = (1/\text{tau})*(\text{CbO}-Y(2))+\text{rb};
38 \text{ w}(3) = (1/\text{tau})*(-Y(3))+\text{rc};
39 w(4) = (1/tau)*(Cm0-Y(4));
40 \text{ 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 \text{ plot2d}(t, x(5,:));
51
52 xtitle ('Figure E9-4.2', 't', 'T');
53 \text{ 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("9.8 data.sci");
5 t = 0:.01:1.5;
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)) \times V / ((Y(1) * 30 + Y(2) * 60 + Y(3) * 20) \times V + 100 * 35);
20 endfunction
21
22 \text{ x=ode}([1;0;0;290],t0,t,f);
23
24
25 scf(1)
26 \quad 11 = x(1, :)
27 \quad 12 = x(2, :)
```

```
28 13=x(3,:)'
29 plot2d(t',[11 12 13]);
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');
```

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("10.3data.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 \text{ rt=-k*kt*ph*pt/(1+kb*pb+kt*pt)};
17 rate=-rt;
18 W(1) = -rt/ft0;
19 endfunction
20 \text{ pt0} = .3 * Po;
21 X = ode([0], w0, w, f);
22
23
24 for i =1:length(X)
     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 \text{ end}
30
31 \text{ m1} = X';
32 \text{ m} 2 = 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 \quad 11 = ph,
41 12=pt'
42 13=pb,
43 plot2d(w',[11 12 13]);
45 xtitle ('Figure E10-3.2', 'w', 'ph,pt,pb');
46 legend(['ph';'pt';'pb']);
```

Scilab code Exa 10.5 clear

```
1 // \operatorname{clear} //
```

```
2 clc
3 clear
4 exec("10.5 data.sci");
5 t = 0:.01:.5;
7 function w=f(t,Y)
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 \text{ Ct0} = 1
21 \text{ ya0=Ca0/Ct0};
22 for i=1:length(t)
     X1(i)=1-(1+ya0)/(1+x(2,i)/Ct0)*x(2,i)/Ca0;
23
24
     end
25
26
27 \quad 11 = x(1, :)
28 \quad 12 = x(2, :)
29 \ 13 = X1;
30 plot2d(t',[11 12 13]);
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 ("9.8 data.sci");
 5 t = 0:.01:.5;
 7 function w=f(t,Y)
 8
 9
    w = zeros(2,1);
10
11 d(X)/d(z}=-ra/U/Ca0
12 \text{ Ka=0.05};
13 Kb = .15;
14 \text{ Pao} = 12;
15 \text{ eps=1};
16 A = 7.6;
17 R = 0.082;
18 T = 400 + 273;
19 Kc = .1;
20 \text{ rho} = 80;
21 \text{ kprime} = 0.0014;
22 D = 1.5;
23 \text{ Uo} = 2.5
24 \quad U:Uo*(1+eps*X)
25 Pa=PBo*(1-X)/(ltepstX)
26 \text{ Pb=Pao*X/(1+eps*X)}
27 \text{ vo} = \text{Uo} * 3.1416 * \text{D} * \text{D} / 4
28 \text{ CaO=PBo/R/T}
29 \text{ Kca=Ka*R*T}
30 \text{ Pc=Pb}
31 \ a=1/(1+At(z/U)**0.S)
32 raprime=at (-kprirne*Pa/(1 t Kat Pa+Kb:1:Pb+Kct Pc
33 ra:rhotraprime
34 endfunction
35
36 \text{ x=ode}([1;.8],t0,t,f);
37 \text{ CaO} = .8;
38 \text{ 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)
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 \text{ vo=Uo*3.1416*D*D/4}
16 Ca0=Pao/R/T
17 Kca=Ka*R*T
18 \text{ 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']);
```

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*CTO*(yAb-yAs)/s;
6 WAZ2=c*DAB*CTO*log((1-yAs)/(1-yAb))/s;
7 disp(WAZ1)
8 disp(WAZ2)
```

Scilab code Exa 11.3 clear

```
1 clc
2 clear
3 exec("11.3 data.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 \operatorname{disp}(\mathrm{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("11.4 data.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("11.5 data.sci")
```

```
5 X2=1-(1/exp((log(1/(1-X1)))*((T2/T1)^(5/12))));
6 disp("X2 =")
7 disp(X2)
```

Distributions of Residence Times for Chemical Reactions

Scilab code Exa 13.8 clear

```
1 // clear //
2 clc
3 clear
4 exec("13.8 data.sci");
5 z = 0:1:200;
7 function w=f(z,x)
9 \quad w = zeros(1,1);
10
11 \quad 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 \quad 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*1am^3 + 5.02846e - 5*1am^2 - .00941*1am
      +.61823-1)
18 ra=-k*ca^2;
19 \text{ if } lam < =70
20
    E = E1
21 else
E = (E2)
23
    end
24 	 if(lam < =70)
25
      F = F 1
    else
26
27
      F = F2
28
       end
       EF=E/(1-F)
29
       w(1) = -(ra/cao + E/(1-F) *x)
30
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 \quad w(1) = ra
24 \text{ w(2)} = \text{rb}
25 \text{ w(3)} = \text{rc}
26 \text{ w (6)} = \text{Y (1)} * \text{E}
27 \text{ w}(7) = \text{Y}(2) * \text{E}
28 \text{ w(8)} = \text{Y(3)} *\text{E}
29 \text{ w } (4) = \text{rd}
30 \text{ w(5)} = \text{re}
31 \text{ w(9)} = \text{Y(4)} * \text{E}
32 \text{ w (10)} = \text{Y (5)} *\text{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,:));
```

Models for Nonideal Reactors

Scilab code Exa 14.3 clear

```
1 // clear //
2 clc
3 clear
5 t = 0:10:200;
7 function w=f(t,Y)
9 \quad 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
14 \text{ alpha=.8}
15 \text{ tau}=40
16 if (t<80)
17 CTe=CTe1
18 else
19 CTe=CTe2
```

```
20 \, \text{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 \text{ X} = \text{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)
     CTe(i) = CTe1(i)
33
34 else
35 CTe(i)=CTe2(i)
36 \text{ end}
37 end
38
39
40 \quad 11 = X(1, :);
41 12 = CTe;
42
43 plot2d(t,[11 12]);
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;
```