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

Created by
Santosh Kumar
B.Tech. + M.Tech
Chemical Engineering
IIT Bombay
College Teacher
Prof. Arun Sadashio Moharir
Cross-Checked by
Prof. Arun Sadashio Moharir

April 15, 2014

[1]Funded 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.

Contents

List of Scilab Codes 4

1 Mole Balances 7

2 Conversion and Reactor Sizing 8

3 Rate Laws and Stoichiometry 14

4 Isothermal Reactor Design 16

5 Collection and Analysis of Rate Data 26

6 Multiple Reactions 29

7 Nonelementary Reaction Kinetics 32

8 Steady State Nonisothermal Reactor Design 35

9 Unsteady State Nonisothermal Reactor Design 44

10 Catalysis and Catalytic Reactors 51

11 External Diffusion Effects on Hetrogeneous Reactions 56

13 Distributions of Residence Times for Chemical Reactions 59

14 Models for Nonideal Reactors 62

List of Scilab Codes

Exa 1.3 clear . . . 7
Exa 2.1 clear . . . 8
Exa 2.2 clear . . . 9
Exa 2.3 clear . . . 9
Exa 2.4 clear . . . 10
Exa 2.5 clear . . . 10
Exa 2.6 clear . . . 11
Exa 2.7 clear . . . 12
Exa 3.5 clear . . . 14
Exa 4.1 clear . . . 16
Exa 4.2 clear . . . 17
Exa 4.4 clear . . . 18
Exa 4.5 clear . . . 18
Exa 4.6 clear . . . 19
Exa 4.7 clear . . . 20
Exa 4.8 clear . . . 21
Exa 4.9 clear . . . 22
Exa 4.10 clear . . . 23
Exa 4.11 clear . . . 24
Exa 5.1 clear . . . 26
Exa 5.2 clear . . . 26
Exa 5.3 clear . . . 27
Exa 5.4 clear . . . 28
Exa 6.6 clear . . . 29
Exa 6.8 clear . . . 30
Exa 7.7 clear . . . 32
Exa 7.8 clear . . . 33
Exa 7.9 clear . . . 33

Exa 8.3 clear . . . 35
Exa 8.4 clear . . . 36
Exa 8.6 clear . . . 37
Exa 8.7 clear . . . 38
Exa 8.9 clear . . . 38
Exa 8.10 clear . . . 40
Exa 8.11 clear . . . 41
Exa 8.12 clear . . . 43
Exa 9.1 clear . . . 44
Exa 9.2 clear . . . 45
Exa 9.3 clear . . . 46
Exa 9.4 clear . . . 47
Exa 9.8 clear . . . 49
Exa 10.3 clear . . . 51
Exa 10.5 clear . . . 53
Exa 10.7 clear . . . 54
Exa 13.8 clear . . . 55
Exa 11.1 clear . . . 56
Exa 11.3 clear . . . 57
Exa 11.4 clear . . . 57
Exa 11.5 clear . . . 58
Exa 13.8 clear . . . 59
Exa 13.9 clear . . . 60
Exa 14.3 clear . . . 62
AP 1 data . . . 64
AP 2 data . . . 64
AP 3 data . . . 64
AP 4 data . . . 64
AP 5 data . . . 64
AP 6 data . . . 65
AP 7 data . . . 65
AP 8 data . . . 65
AP 9 data . . . 66
AP 10 data . . . 66
AP 11 data . . . 66
AP 12 data . . . 66
AP 13 data . . . 67
AP 14 data . . . 67

AP 15 data 67
AP 16 data 67
AP 17 data 67
AP 18 data 68
AP 19 data 68
AP 20 data 69
AP 21 data 69
AP 22 data 69
AP 23 data 69
AP 24 data 69
AP 25 data 70
AP 26 data 70
AP 27 data 70
AP 28 data 70
AP 29 data 70
AP 30 data 70
AP 31 data 71
AP 32 data 71
AP 33 data 71
AP 34 data 72
AP 35 data 72
AP 36 data 72
AP 37 data 72
AP 38 data 73
AP 39 data 73
AP 40 data 73
AP 41 data 73
AP 42 data 74
AP 43 data 74
AP 44 data 74
AP 45 data 75
AP 46 data 75
AP 47 data 75

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("2.1data.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")
```

---

check Appendix AP 46 for dependency:

2_2.sci

Scilab code Exa 2.2 clear

```
1  //clear//
2  clc
3  clear
4  exec("2.2data.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("2.3data.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.")
```

---

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

```
//clear//
clc
clear
exec("2.5data.sci");


V1 = FA0*X1*(1/-rA);
V2 = FA0*(X2-X1)*(1/-rA2);
V = FA0*X*(1/-rA2);
disp("V1 =")
disp(V1)
disp("dm^3")
disp("V2 =")
disp(V2)
disp ("dm^3")
disp("V =")
disp(V)
disp ("dm^3")
```

---

check Appendix AP 42 for dependency:

2_6.sce

Scilab code Exa 2.6 clear

```
//clear//
clc
clear all
exec("2.6data.sci");


X1 = X(1:5);
p1 = p(1:5);
V1 = FA0*inttrap(X1,p1)
X2 = X(5:9);
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("3.5data.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

check Appendix AP 39 for dependency:

4_1.sci

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")
```

check Appendix AP 36 for dependency:

4_2.sci

Scilab code Exa 4.2 clear

```
1  //clear//
2  clc
3  clear
4  exec("4.2data.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
```

```
G = m/Ac;
bita0 = (G*(1-phi)/(gc*rho*Dp*phi^3))*((150*(1-phi)*
   mu/Dp)+1.75*G);
bita0 = bita0/(144*14.7);//atm/ft
P = ((1-(2*bita0*L/P0))^.5)*P0;
deltaP = P0 - P;

disp("deltaP")
disp(deltaP)
disp("atm")
```

check Appendix AP 33 for dependency:

4_6.sci

Scilab code Exa 4.6 clear

```
//clear//
clc
clear
exec("4.6data.sci");

FT0 = FA0+FB0+FI;
yA0 = FA0/FT0;
e = yA0*(1-.5-1);
PA0 = yA0*P0;
kdes = k*PA0*(1/2)^(2/3);
alpha = 2*bita0/(Ac*(1-phi)*rhoc*P0);
W = (1 - (1-(3*alpha*FA0/(2*kdes))*((1+e)*log(1/(1-X
   ))-e*X))^(2/3))/alpha;


disp("W")
disp(W)
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 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
```

```
l1=x(1,: )'
l2=x(2,: )'
l3=F'
plot2d(W',[l1 l2 l3]);

xtitle( 'Figure E4-7.2', 'w', 'x,y,z' ) ;
legend(['x';'y';'f']);
```

---

check Appendix AP 31 for dependency:

4_8.sci

Scilab code Exa 4.8 clear

```
//clear//
clc
clear
exec("4.8data.sci");
Z = 0:1:12;
function w=f(Z,Y)

 w=zeros(2,1);
 Ac= 3.14*((R^2)-(Z-L)^2);
 Ca = Ca0*(1-Y(1))*Y(2)/(1+Y(1));
 ra =kprime*Ca*rhocat*(1-phi);
 G= m/Ac;
 V =3.14*(Z*(R^2)-(1.3*(Z-L)^3)-(1/3)*L^3)
 bita = (98.87*G+25630*G^2)*0.01;
 W=rhocat*(1-phi)*V
w(1)= -ra*Ac/FA0
w(2) = -bita/P0/(Y(2)*(1+Y(1)));
endfunction


x=ode([0;1],Z0,Z,f);
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
```

```
exec("5.2data.sci");
 for i =1:length(t)
g(i) =log(2*P0/(3*P0-P(i)));
end
plot2d(t,g);

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

```
//Clear//
clc
clear
exec("5.3data.sci");

x=log(CHCl);
y=log(-rHCl);
plot2d(x,y);

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;
```

```
 Cf =2*f(6)/ft;
w(1)= 1.25*r1a+.75*r2a+r3b;
 w(2) = r1a+r2a+2*r4c/3;
 w(3) = -r1a+2*r3b+r4c;
 w(4) =-1.5*r1a-1.5*r2a-r4c;
 w(5) =.5*r2a-5*r4c/6;
 w(6) = -2*r3b;

endfunction

x=ode([9;9;0;0;0;0],v0,v,FF);

plot2d(v,x(1,:)/10,rect=[1,0,10,1.5]); //B
plot2d(v,x(2,:)/10,rect=[1,0,10,1.5]); //A
plot2d(v,x(3,:)/10,rect=[1,0,10,1.5]); //C
plot2d(v,x(4,:)/10,rect=[1,0,10,1.5]);
plot2d(v,x(5,:)/10,rect=[1,0,10,1.5]);
plot2d(v,x(6,:)/10,rect=[1,0,10,1.5]);
xtitle('FigureE');
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 = 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']);
```

check Appendix AP 16 for dependency:

8_6.sci

Scilab code Exa 8.6 clear

```
1  //clear//
2  clc
3  clear
4  exec("8.6data.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
   )' ) ;
```

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+
      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;
```

```
Kp=exp(42311/R/Y(3)-11.24);
if(Y(2)< =.05)

  ra=(-k*(.848-.012/(Kp**2)));
else
  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)));
end

w(1)=(-1.12*10**(-8)*(1-.055*Y(2))*Y(3))*(5500*visc
   +2288)/Y(1) ;
w(2)=-(ra)/fao ;
w(3)=(5.11*(Ta-Y(3))+(-ra)*(-deltah) )/(fao*(summ+Y
   (2)*dcp))
endfunction

X=ode([2;0;1400],W0,W,f);

plot2d(W,X(1,:));
plot2d(W,X(3,:));
```

---

check Appendix AP 20 for dependency:

```
8__11.sci
```

Scilab code Exa 8.11 clear

```
//clear//
clc
clear
exec("8__11.sci");
V = 0:.01:1;

function w=f(V,Y)

```

```
 w =zeros(4,1);

k1a=10*exp(4000*((1/300)-(1/Y(4))));
k2a=.09*exp(9000*((1/300)-(1/Y(4))))

Ft=Y(1)+Y(2)+Y(3);

Ca=Cto*(Y(1)/Ft)*(To/Y(4))
Cb=Cto*(Y(2)/Ft)*(To/Y(4))
Cc=Cto*(Y(3)/Ft)*(To/Y(4))
r1a=-k1a*Ca;
r2a=-k2a*Ca^2;

w(1)=r1a+r2a;
w(2)=-r1a;

w(3)=-r2a/2;
w(4)=(4000*(373-Y(4))+(-r1a)*20000+(-r2a)*60000)
   /(90*Y(1)+90*Y(2)+180*Y(3));
endfunction

x=ode([100;0;0;423],V0,V,f);

scf(1)
plot2d(V,x(4,:));

xtitle( 'Figure E8-11.1', 'V', 'T' ) ;

scf(2)

l1=x(1,: )'
l2=x(2,: )'
l3=x(3,: )'
plot2d(V',[l1 l2 l3]);

xtitle( 'Figure E8-11.2', 'V', 'Fa,Fb,Fc' ) ;
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("9.1data.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
```

```
w(2)=(-ra)*U/Nao
endfunction

x=ode([467.992;0.0423],t0,t,f);


plot2d(t,x(1,:));

xtitle( 'Figure E9-2.2', 't ', 'T (oC)' ) ;
```

check Appendix AP 12 for dependency:

9_3.sci

Scilab code Exa 9.3 clear

```
//clear//
clc
clear
exec("9.3data.sci");
t = 0:1:360;

function w=f(t,Y)

 w =zeros(5,1);

k=.39175*exp(5472.7*((1/273)-(1/Y(4))));
Cd=Y(3);

Kc=10^(3885.44/Y(4))
V=Vi+v0*t;
Fb0=Cb0*v0;
ra=-k*((Y(1)*Y(2))-((Y(3)*Cd)/Kc));
Na=V*Y(1)
Nb=V*Y(2)
Nc=V*Y(3)
```

```
rb=ra
rc=-ra
Nd=V*Cd
rate=-ra
NCp=cp*(Nb+Nc+Nd+Y(5))+cpa*Na;
w(1)=ra-(v0*Y(1))/V;
w(2) =rb+(v0*(Cb0-Y(2))/V);
w(3) =rc- (Y(3)*v0)/V;
w(4)= (UA*(Ta-Y(4))-Fb0*cp*(1+55)*(Y(4)-T0)+ra*V*dh)
   /NCp
w(5) =v0*Cw0
endfunction

x=ode([5;0.0001;00.0001;300;6.14],t0,t,f);
scf(1)
plot2d(t,x(4,:));

xtitle( 'Figure E9-3.1', 't', 'T' ) ;

scf(2)
l1=x(1,: )'
l2=x(2,: )'
l3=x(3,: )'
plot2d(t',[l1 l2 l3]);

xtitle( 'Figure E9-3.2', 't', 'Ca,Cb,Cc' ) ;
legend(['Ca';'Cb';'Cc']);
```

---

check Appendix AP 11 for dependency:

9_4.sci

Scilab code Exa 9.4 clear

```
//clear//
clc
```

```
clear
//exec("9.3data.sci");
t = 0:.0001:4;
t0=0;
function w=f(t,Y)

 w =zeros(5,1);

Fa0=80;
T0=75;
V=(1/7.484)*500;
UA=16000;
Ta1=60;
k=16.96e12*exp(-32400/1.987/(Y(5)+460));
Fb0=1000;
Fm0=100;
mc=1000;
ra=-k*Y(1);
rb=-k*Y(1);
rc=k*Y(1) ;
Nm=Y(4)*V;
Na=Y(1)*V;
Nb=Y(2)*V;
Nc=Y(3)*V;
ThetaCp=35+(Fb0/Fa0)*18+(Fm0/Fa0)*19.5;
v0=(Fa0/0.923)+(Fb0/3.45)+(Fm0/1.54);
Ta2=Y(5)- (Y(5)-Ta1)*exp (-UA/(18*mc));
Ca0=Fa0/v0
Cb0=Fb0/v0
Cm0=Fm0/v0
Q=mc*18*(Ta1-Ta2);
tau=V/v0;
NCp=Na*35+Nb*18+Nc*46+Nm*13.5;
w(1)=(1/tau)*(Ca0-Y(1))+ra;
w(2)=(1/tau)*(Cb0-Y(2))+rb;
w(3)=(1/tau)*(-Y(3))+rc;
w(4) =(1/tau)*(Cm0-Y(4));
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;
```

```
rt=-k*kt*ph*pt/(1+kb*pb+kt*pt);
rate=-rt;
W(1)=-rt/ft0;
endfunction
pt0=.3*Po;
X=ode([0],w0,w,f);


for i =1:length(X)
  y(1,i)=(1-alpha*w(1,i))^.5;
ph(1,i)=pt0*(1.5-X(1,i))*y(1,i);
pt(1,i)=pt0*(1-X(1,i))*y(1,i);
pb(1,i)=2*pt0*X(1,i)*y(1,i)
end

m1 = X';
m2=y';
scf(1)
plot2d(w',[m1 m2]);

xtitle( 'Figure E10-3.1', 'w', 'x,y' ) ;
legend(['x';'y']);

scf(2)
l1=ph'
l2=pt'
l3=pb'
plot2d(w',[l1 l2 l3]);

xtitle( 'Figure E10-3.2', 'w', 'ph,pt,pb' ) ;
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("10.5data.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
```

```
l1=x(1,: )'
l2=a(1,: )'

plot2d(z',[l1 l2]);

xtitle( 'Figure E10-7.1', 'z', 'X,a' ) ;
legend(['X';'a']);
```

Scilab code Exa 13.8 clear

```
k=0.1
cao=8;
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")
```

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

check Appendix AP 3 for dependency:

11_5.sci

Scilab code Exa 11.5 clear

```
//clear//
clc
clear
exec("11.5data.sci")
X2=1-(1/exp((log(1/(1-X1)))*((T2/T1)^(5/12))));
disp("X2 =")
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+1.854;
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  H0C= -226000;
3  H0B = -123000;
4  H0A = -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 H0NH3 = -11020; // cal/moleN2
2 H0H2 = 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 PCO= [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 PCO= [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 FB0 = 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

```
k= 2.2;
v00 = .05;
Cb0 = .025;
v0 = 5;
Ca0 = .05;
t0 = 0;
```

Scilab code AP 38 data

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

Scilab code AP 39 data

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

Scilab code AP 40 data

```
CA0 = 10;
CB0 = 2;
X = 0.2;
X1=0.9
```

Scilab code AP 41 data

```
FA0 = 0.867; // mol/s
X1 = 0.5;
X2 = 0.8;
rA2 = -(1/800);
X = [0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8]';
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("2.6data.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 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
```