Scilab Code for Elements of chemical Reaction Engineering by H. Scott Fogler[1]

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Mole Balances

1.1 Discussion

When executing the code from the editor, use the 'Execute File into Scilab'tab and not the 'Load in Scilab'tab. The .sci files of the respective problems contain the input parameters of the question

1.2 Scilab Code

Example 1.3 1.3data.sci

```
k = 0.23; //min^-1
v0 = 10;//dm^3/min
```

Example 1.3 1.3.sce

```
clc
clear all
exec("1.3data.sci");

//CA = 0.1*CA0;
V = (v0/k)*log(1/0.1);
disp("V =")
disp(V)
disp ("dm^3")
```

Chapter 2

Conversion and Reactor Sizing

2.1 Discussion

When executing the code from the editor, use the 'Execute File into Scilab'tab and not the 'Load in Scilab'tab. The .sci files of the respective problems contain the input parameters of the question

2.2 Scilab Code

Example 2.1 2.1data.sci

```
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
```

Example 2.1 2.1.sce

```
1 clc
2 clear all
3 exec("2.1data.sci");
4 CA0=(yA0*P0)/(R*T0);
5 FA0 = CA0*v0;
6 disp("CA0 =")
```

```
disp(CA0)
disp ("mol/dm^3")
disp("FA0 =")
disp(FA0)
disp("mol/s")
```

Example 2.2 2.2data.sci

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

Example 2.2 2.2.sce

```
clc
clear all
exec("2.2data.sci");
CA0=(yA0*P0)/(R*T0);
FA0 = CA0*v0;
V = FA0*X*(1/-rA)

disp("FA0 =")
disp(FA0)
disp("mol/s")
disp("V =")
disp(V)
disp ("dm^3")
```

Example 2.3 2.3data.sci

```
P0 = 10; //atm
yA0 = 0.5;
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
```

Example 2.3 2.3.sce

```
1 clc
2 clear all
3 exec("2.3data.sci");
4 CA0=(yA0*P0)/(R*T0);
5 FA0 = CA0*v0;
6 //V = FA0*X*(1/-rA)
7
8 V = FA0*inttrap(X,p)
9 disp("FA0 =")
10 disp(FA0)
11 disp("mol/s")
12 disp("V =")
13 disp(V)
14 disp ("dm^3")
15 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.")
```

Example 2.4 2.4data.sci

```
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
```

Example 2.4 2.4.sce

```
clc
clear all
exec("2.4data.sci");


VCSTR = FA0*X(7)*(1/-rAat);
VPFR = FA0*inttrap(X,p)
disp("VCSTR =")
disp(VCSTR)
disp("dm^3")
disp("VPFR =")
disp(VPFR)
disp ("dm^3")
```

Example 2.5 2.5data.sci

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

Example 2.5 2.5.sce

```
clc
clear all
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)
```

```
14 disp ("dm^3")
15 disp("V =")
16 disp(V)
17 disp ("dm^3")
```

Example 2.6 2.6data.sci

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

Example 2.6 2.6.sce

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

Example 2.7 2.7data.sci

```
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
```

Example 2.7 2.7.sce

```
clc
clear all
exec("2.7data.sci");


X = X(1:6);
p = p(1:6);
V1 = FA0*inttrap(X,p);
V2 = FA0*(X2-X1)*(1/-rA2);
V=V1+V2;
disp("V1 =")
disp(V1)
disp("dm^3")
disp("V2 =")
disp(V2)
disp ("dm^3")
disp("V =")
disp(V)
disp ("dm^3")
```

Chapter 3

Rate Laws and Stoichiometry

3.1 Discussion

When executing the code from the editor, use the 'Execute File into Scilab'tab and not the 'Load in Scilab'tab. The .sci files of the respective problems contain the input parameters of the question

3.2 Scilab Code

Example 3.5 3.5data.sci

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

Example 3.5 3.5.sce

```
1 clc
2 clear all
3 exec("3.5data.sci");
4 CD=CA0*(X/3);
5 CB=CA0*((CB0/CA0)-(X/3));
6 CD1=CA0*(X1/3);
7 CB1=CA0*((CB0/CA0)-(X1/3));
```

```
disp("For 20% conversion")
disp("CD =")
disp(CD)
disp ("mol/dm^3")
disp("CB =")
disp(CB)
disp("mol/dm^3")
disp("For 90% conversion")
disp("CD =")
disp(CD1)
disp ("mol/dm^3")
disp("CB =")
disp(CB1)
disp("mol/dm^3")
```

Chapter 4

Isothermal Reactor Design

4.1 Discussion

When executing the code from the editor, use the 'Execute File into Scilab'tab and not the 'Load in Scilab'tab. The .sci files of the respective problems contain the input parameters of the question

4.2 Scilab Code

Example 4.1 4.1data.sci

```
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;
```

Example 4.1 4.1.sce

```
clc
clear all
exec("4.1data.sci");

x=t;
y =((CA0-CC)/CA0);

yi=interpln([x;y],x);
```

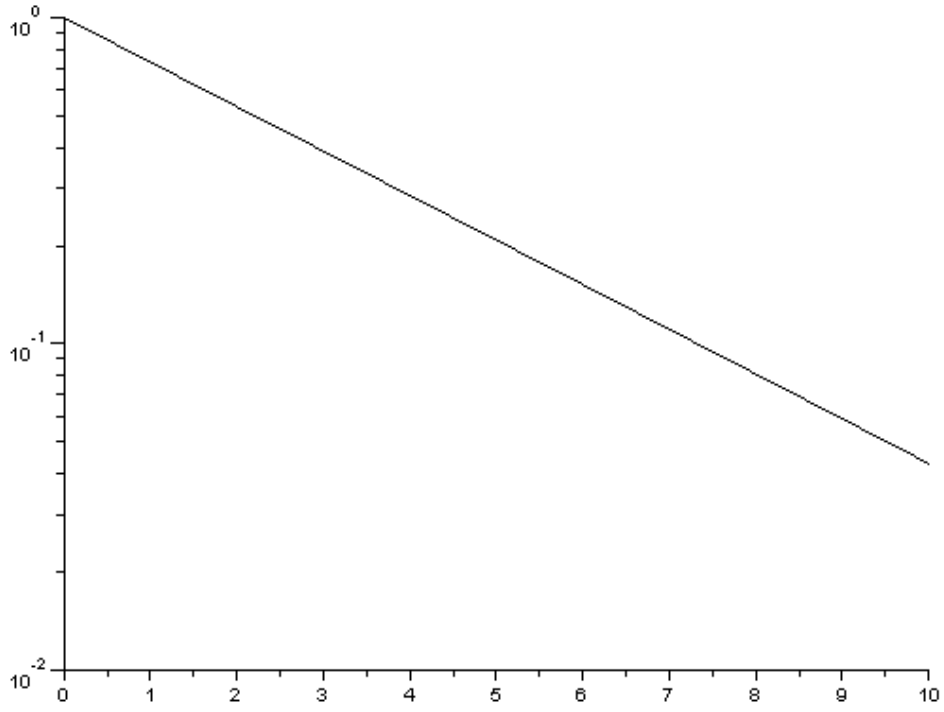

Figure 4.1: Output graph of S 4.1

```
9  plot2d(x,y,logflag='nl');
10
11 k = log(y(9)/y(2))/(t(9)-t(2));
12
13
14 disp("k =")
15 disp(k)
16 disp ("min^-1")
```

Example 4.2 4.2data.sci

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

Example 4.2 4.2.sce

```
clc
clear all
exec("4.2data.sci");

 FA0 = FC/X;
 vA0 = FA0/CA01;
 vB0 = vA0;
 v0 = vA0+vB0;
 V = v0*X/(k*(1-X));

 // CSTR in parallel
 V1 = 800/7.48;

 Tau =V1/(v0/2);
 Da= Tau*k;
 Xparallel = Da/(1+Da)

 // CSTR in series
 Tau =V1/v0;
 n=2;
 Xseries = 1- (1/(1+Tau*k)^n);

disp("Reactor volume")
disp(V)
disp ("ft^3")
disp("CSTR in parallel X =")
disp(Xparallel)
disp("CSTR in series X =")
disp(Xseries)
```

Example 4.4 4.4data.sci

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

Example 4.4 4.4.sce

```
clc
clear all
exec("4.4data.sci");

 FA0 = FB/X;
 CA0 = yA0*P0/(R*T0);
 R = 1.987;
 k2 = k1*exp((E/R)*((1/T1)-(1/T2)));
 V =( FA0/(k2*CA0))*((1+e)*log(1/(1-X))-e*X);

disp("Reactor volume")
disp(V)
disp("ft^3")
```

Example 4.5 4.5data.sci

```
Ac = 0.01414; // ft^2
m = 104.4; // lbm/h
mu = 0.0673; // lbm/ft.h
Dp = 0.0208; //ft
gc = 4.17e8; // lbm.ft/lbf.h^2
phi = 0.45;
rho = 0.413; // lbm/ft^3
P0 = 10; // atm
```

```
9 L = 60; // ft
```

Example 4.5 4.5.sce

```
1 clc
2 clear all
3 exec("4.5data.sci");
4
5 G = m/Ac;
6 bita0 = (G*(1-phi)/(gc*rho*Dp*phi^3))*((150*(1-phi)*
    mu/Dp)+1.75*G);
7 bita0 = bita0/(144*14.7);//atm/ft
8 P = ((1-(2*bita0*L/P0))^.5)*P0;
9 deltaP = P0 - P;
10
11 disp("deltaP")
12 disp(deltaP)
13 disp("atm")
```

Example 4.6 4.6data.sci

```
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;
```

Example 4.6 4.6.sce

```
1 clc
2 clear all
3 exec("4.6data.sci");
```

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

Example 4.7 4.7data.sci

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

Example 4.7 4.7.sce

```
1  clc
2  clear all
3  exec("4.7data.sci");
4   W = 0:1:60;
5  function w=f(W,Y)
6
7  w=zeros(2,1);
8  w(1)= (kprime/FA0)*((1-Y(1))/(1+e*Y(1)))*Y(2);
9  w(2) = -alpha*(1+e*Y(1))/(2*Y(2));
10 endfunction
11
12
13 x=ode([0;1],W0,W,f);
```

```
for i= 1:61
  F(i) = (1+e*x(1,i))/x(2,i);
end
F= F';
for i= 1:61
  rate(i) = (kprime)*((1-x(1,i))/(1+e*x(1,i)))*x(2,i
     );
end
rate =rate';

scf(1)
plot2d(W,rate);
xtitle( 'Figure E4-7.1 Reaction rate porfile down
   the PBR', 'w', 'rate' ) ;
scf(2)

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']);
```

Example 4.8 4.8data.sci

```
FA0 = 440;
P0 = 2000;
Ca0 = .32;
R = 30;
phi = .4;
kprime = 0.02; //lb.mol/atm.lb cat.h
L = 27;
rhocat = 2.6;
m=44;

alpha = 0.0166;
```

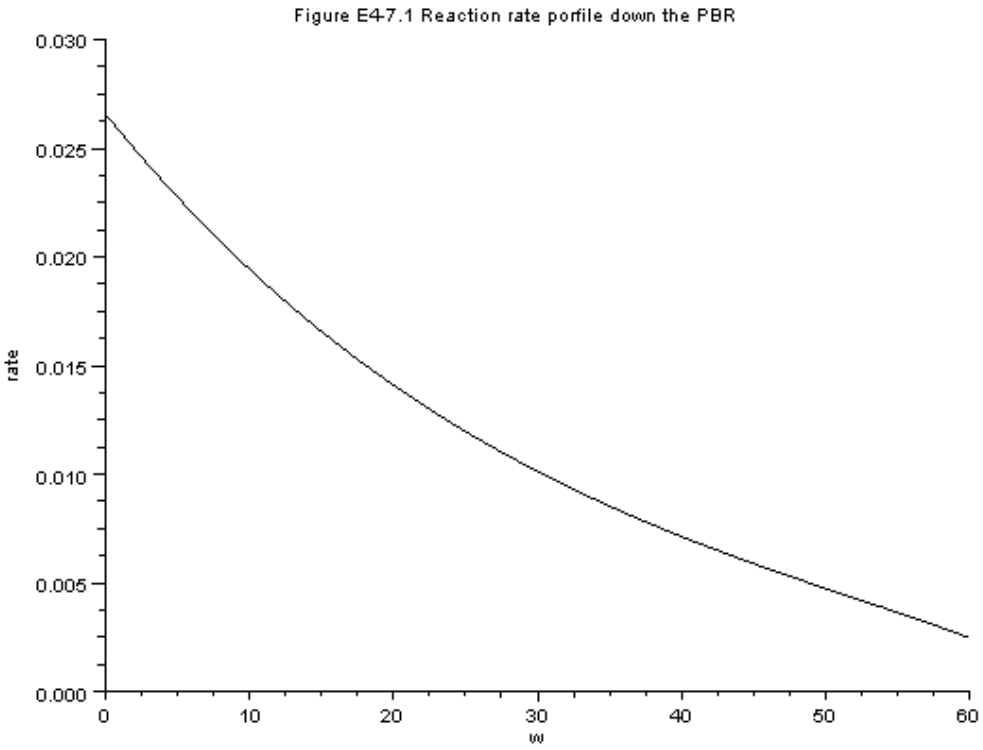

Figure 4.2: Output graph of S 4.7

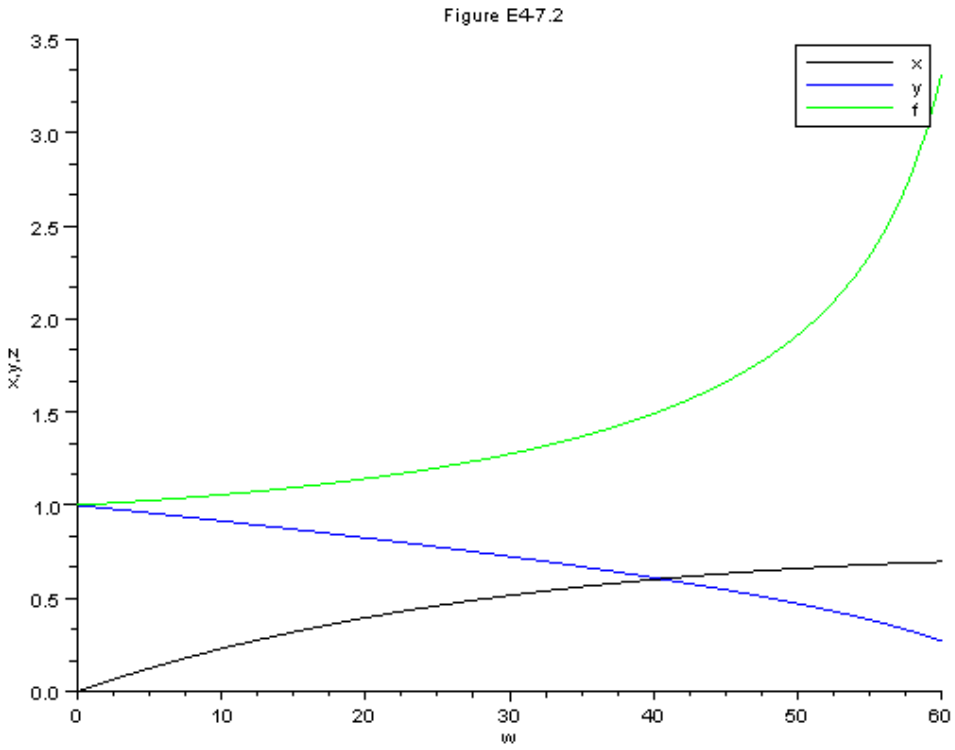

Figure 4.3: Output graph of S 4.7

```
e = -0.15;
Z0 = 0;
```

Example 4.8 4.8.sce

```
clc
clear all
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)
  V(1,i) =3.14*Z(1,i)*((R^2)-(Z(1,i)-L)^2)
   W1(1,i)=rhocat*(1-phi)*V(1,i)
end

l1=x(1,:)'
l2=x(2,:)'

plot2d(W1',[l1 l2]);

xtitle( 'Figure E4-8.2', 'w', 'x,y' ) ;
legend(['x';'y']);
```

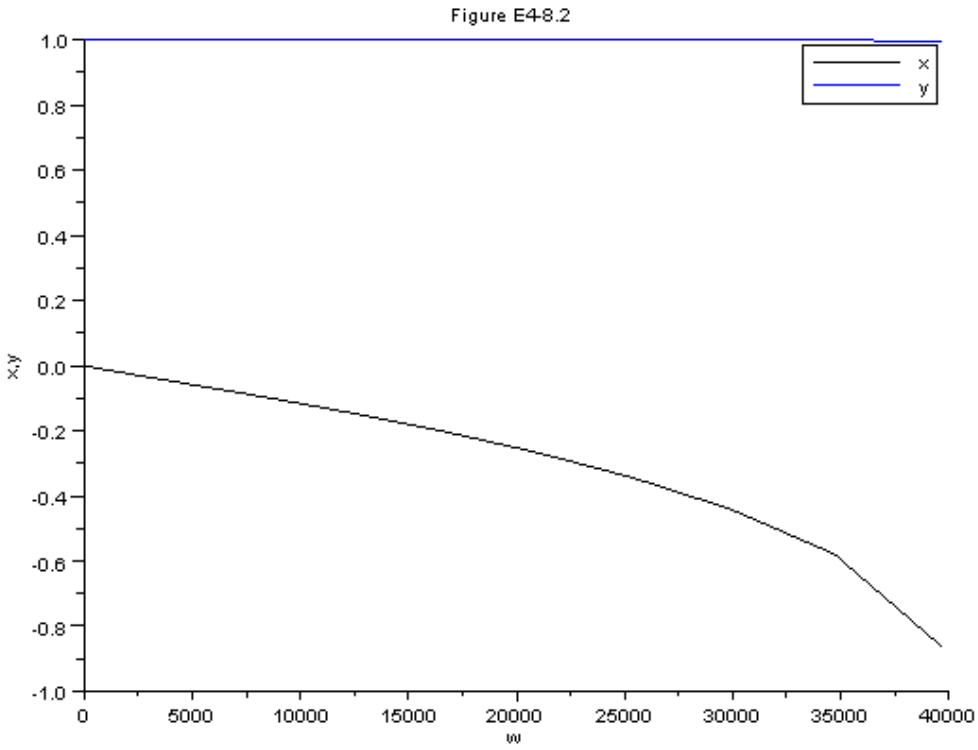

Figure 4.4: Output graph of S 4.8

Example 4.9 4.9data.sci

```
ka = 2.7;
kc = 1.2;
Ct0 = .1;
fa0 =10;
V0 = 0;
```

Example 4.9 4.9.sce

```
clc
clear all
exec("4.9data.sci");
 V = 0:1:100;
function w=f(V,fa)

 w=zeros(1,1);
 ft =2*(fa0-fa(1))
 Ca = Ct0*fa(1)/ft;
 fb = 2*(fa0-fa(1));
 Cb = Ct0*fb/ft;
w(1)= -ka*(Ca-(Cb^2)/kc)

endfunction


x=ode([9.99],V0,V,f);

for i= 1:101
   fb(1,i) = 2*(fa0-x(1,i));
end
l1=x';
l2=fb';

plot2d(V',[l1 l2]);

xtitle( 'Figure E4-9.1 Molar flow rate profiles', 'V
   ', 'fa,fb' ) ;
```

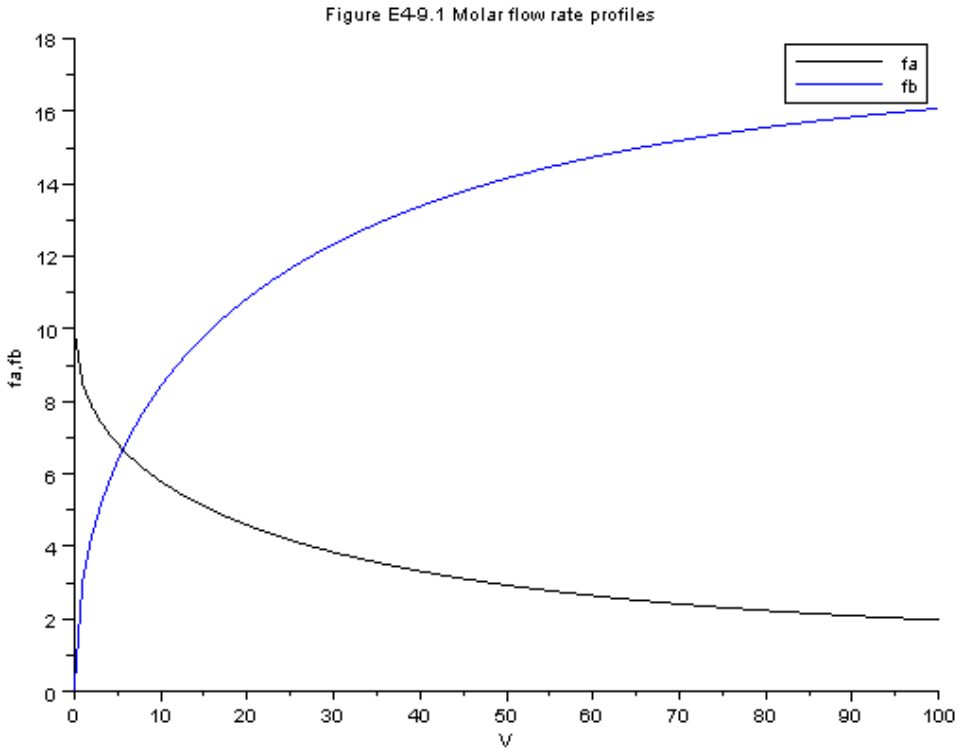

Figure 4.5: Output graph of S 4.9

```
28 legend(['fa';'fb']);
```

Example 4.10 4.10data.sci

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

Example 4.10 4.10.sce

```
clc
clear all
exec("4.10data.sci");
 V = 0:1:500;
function w=f(V,F)

 w=zeros(3,1);

 Ft=F(1)+F(2)+F(3);
 ra = -k*Ct0*((F(1)/Ft)-(Ct0/kc)*(F(2)/Ft)*(F(3)/Ft)
    );
 w(1)= ra;
 w(2) = -ra-kc*Ct0*(F(2)/Ft)
 w(3) = -ra;

endfunction


x=ode([10;0;0],V0,V,f);

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

xtitle( 'Figure E4-10.2', 'V', 'Fa,Fb,Fc' ) ;
legend(['Fa';'Fb';'Fc']);
```

Example 4.11 4.11data.sci

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

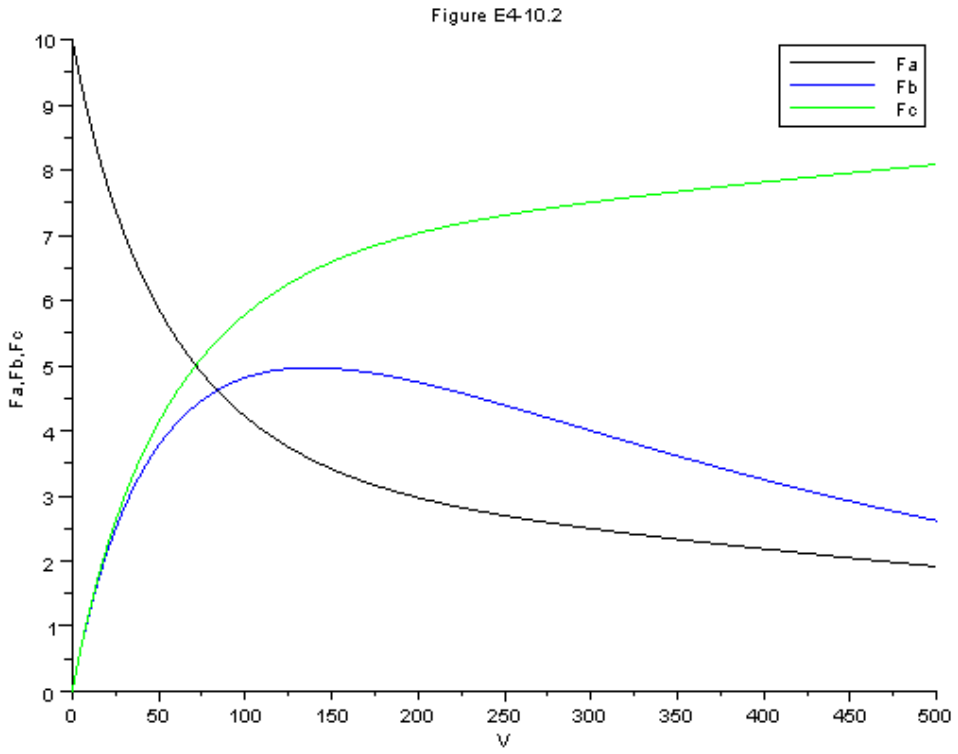

Figure 4.6: Output graph of S 4.10

Example 4.11 4.11.sce

```
clc
clear all
exec("4.11data.sci");
 t = 0:1:500;
function w=f(t,C)

 w =zeros(4,1);

 v = v0+v00*t;
 w(1)= -k*C(1)*C(2)-v00*C(1)/v;
 w(2) = -k*C(1)*C(2)+v00*(Cb0-C(2))/v;
 w(3) = k*C(1)*C(2)-v00*C(3)/v;
 w(4) = k*C(1)*C(2)-v00*C(4)/v;

endfunction


x=ode([.049;0;0;0],t0,t,f);
l1=x(1,:)'
l2=x(2,:)'
l3=x(3,:)'
for i = 1:length(t)
  rate(1,i)=k*x(1,i)*x(2,i)
  end
scf(1)
plot2d(t',[l1 l2 l3]);

xtitle( 'Figure E4-11.1 Concentration-time
   trajectories', 't', 'Ca,Cb,Cc' ) ;
legend(['Ca';'Cb';'Cc']);
scf(2)
plot2d(t,rate)
xtitle( 'Figure E4-11.2 Reaction rate-time
   trajectories', 't', 'Reaction Rate(mols dm^3)' )
   ;

```

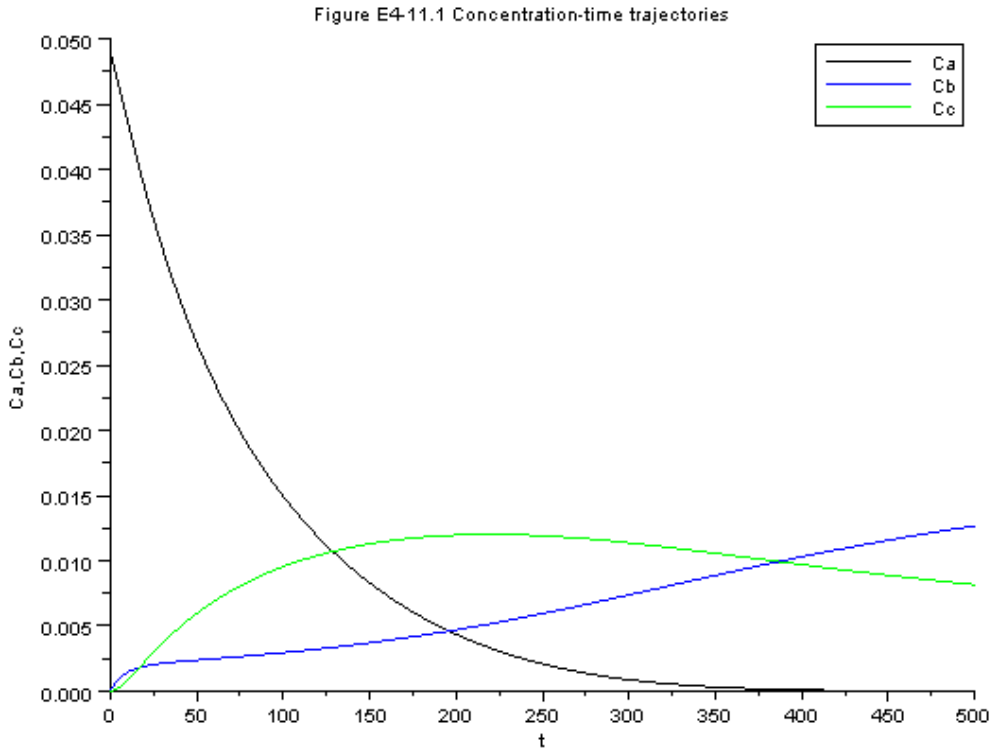

Figure 4.7: Output graph of S 4.11

34
35
36
37 ’V

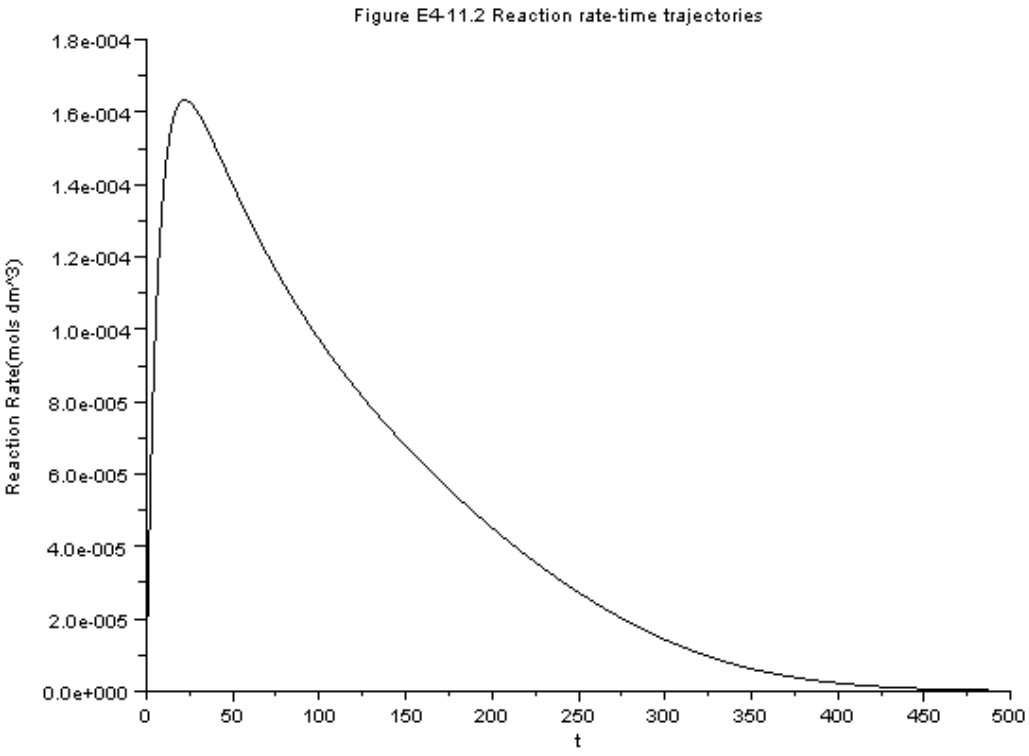

Figure 4.8: Output graph of S 4.11

Chapter 5

Collection and Analysis of Rate Data

5.1 Discussion

When executing the code from the editor, use the 'Execute File into Scilab'tab and not the 'Load in Scilab'tab. The .sci files of the respective problems contain the input parameters of the question

5.2 Scilab Code

Example 5.2 5.2data.sci

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

Example 5.2 5.2.sce

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

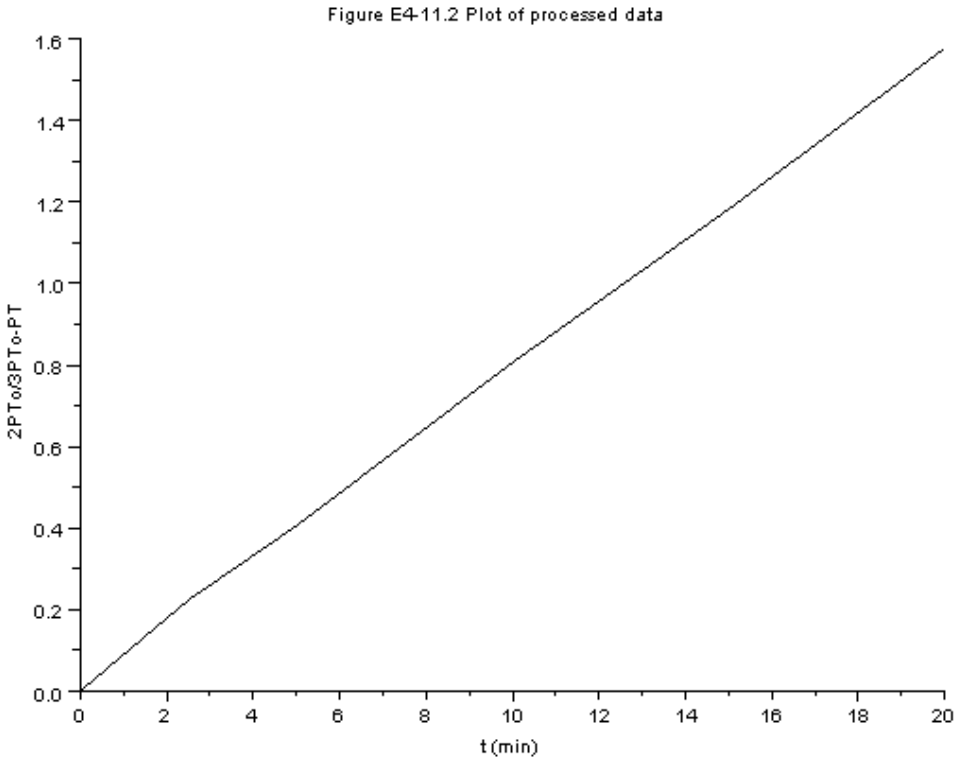

Figure 5.1: Output graph of S 5.2

```
7 plot2d(t,g);
8
9 xtitle( 'Figure E4-11.2 Plot of processed data', 't
    (min)', '2PTo/3PTo-PT' ) ;
```

Example 5.3 5.3data.sci

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

Example 5.3 5.3.sce

```
clc
clear all
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)' ) ;
```

Example 5.4 5.4data.sci

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

Example 5.4 5.4.sce

```
clc
clear all
exec("5.4data.sci");

rCH4 = (v0/W)*CCH4;x
x=log(PCO);
y = log(rCH4)
alpha= (y(3)-y(2))/(x(3)-x(2));
//plot2d(x,y)
disp("alpha")
disp(alpha)
```

Chapter 6

Multiple Reactions

6.1 Discussion

When executing the code from the editor, use the 'Execute File into Scilab'tab and not the 'Load in Scilab'tab. The .sci files of the respective problems contain the input parameters of the question

6.2 Scilab Code

Example 6.6 6.6data.sci

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

Example 6.6 6.6.sce

```
1 clc
2 clear all
3 exec("6.6data.sci");
4  t = 0:.01:.5;
5 function w=f(t,c)
6
7  w =zeros(3,1);
8
```

```
r1 = -k1*c(2)*c(1)^.5;
r2 = -k2*c(3)*c(1)^.5;
 w(1)= r1+r2;
 w(2) = r1;
 w(3) = -r1+r2;

endfunction

x=ode([.021;.0105;0],t0,t,f);

l1=x(1,:)'
l2=x(2,:)'
l3=x(3,:)'

plot2d(t',[l1 l2 l3]);

xtitle( 'Figure E6-6.1', 'Tau (hr)', 'Concentration
   (lb mol/ft^3') ;
legend(['CH';'CM';'CX']);
```

Example 6.8 6.8data.sci

```
v0 =0;
```

Example 6.8 6.8.sce

```
clc
clear all
exec("6.8data.sci");
 v = 0:.1:10;
function w =FF(v,f)

 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;
 r2a = -2*4*(f(1)/ft)*(f(2)/ft);
 r4c = -5*3.175*(f(3)/ft)*(f(1)/ft)^(2/3);
```

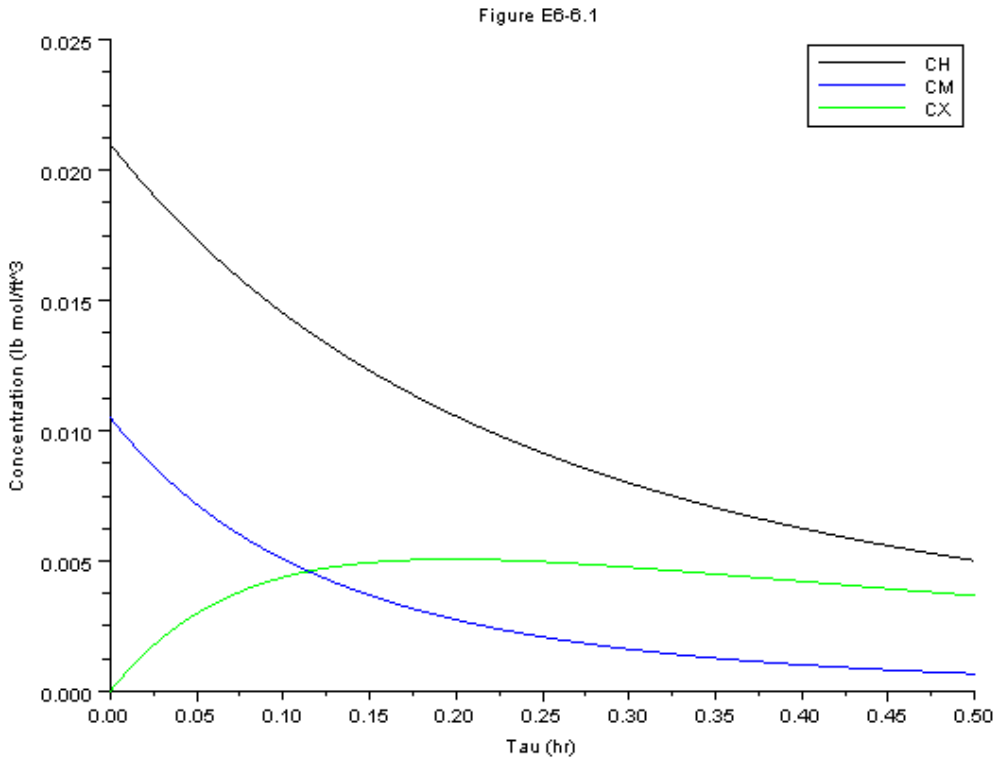

Figure 6.1: Output graph of S 6.6

```
12   r3b = -10*8*((f(3)/ft)^2)*(f(2)/ft);
13   Ca =2*f(1)/ft;
14   Cb =2*f(2)/ft;
15   Cc =2*f(3)/ft;
16   Cd =2*f(4)/ft;
17   Ce =2*f(5)/ft;
18   Cf =2*f(6)/ft;
19  w(1)= 1.25*r1a+.75*r2a+r3b;
20   w(2) = r1a+r2a+2*r4c/3;
21   w(3) = -r1a+2*r3b+r4c;
22   w(4) =-1.5*r1a-1.5*r2a-r4c;
23   w(5) =.5*r2a-5*r4c/6;
24   w(6) = -2*r3b;
25
26  endfunction
27
28  x=ode([9;9;0;0;0;0],v0,v,FF);
29
30  plot2d(v,x(1,:)/10,rect=[1,0,10,1.5]); //B
31  plot2d(v,x(2,:)/10,rect=[1,0,10,1.5]); //A
32  plot2d(v,x(3,:)/10,rect=[1,0,10,1.5]); //C
33  plot2d(v,x(4,:)/10,rect=[1,0,10,1.5]);
34  plot2d(v,x(5,:)/10,rect=[1,0,10,1.5]);
35  plot2d(v,x(6,:)/10,rect=[1,0,10,1.5]);
36  xtitle('FigureE');
37  legend (['B';'A';'C';'D';'E';'F']);
```

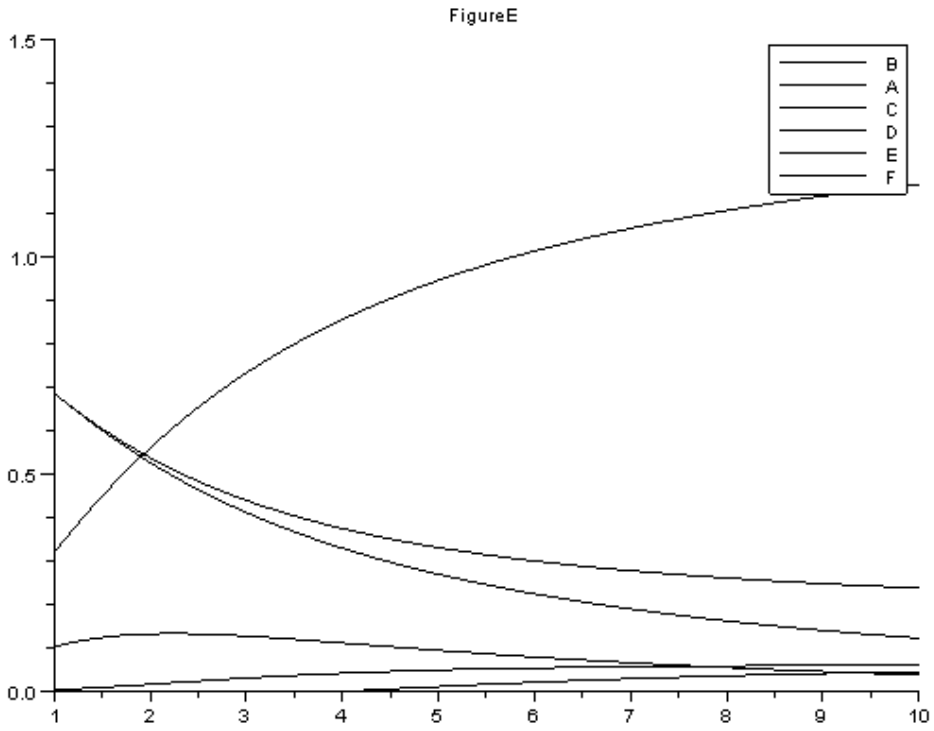

Figure 6.2: Output graph of S 6.8

Chapter 7

Nonelementary Reaction Kinetics

7.1 Discussion

When executing the code from the editor, use the 'Execute File into Scilab'tab and not the 'Load in Scilab'tab. The .sci files of the respective problems contain the input parameters of the question

7.2 Scilab Code

Example 7.7 7.7data.sci

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

Example 7.7 7.7.sce

```
1 clc
2 clear all
3 exec("7.7data.sci");
4 for i=1:length(Curea)
5 x(i)= 1/Curea(i);
6 y(i) = 1/(-rurea(i));
7 end
```

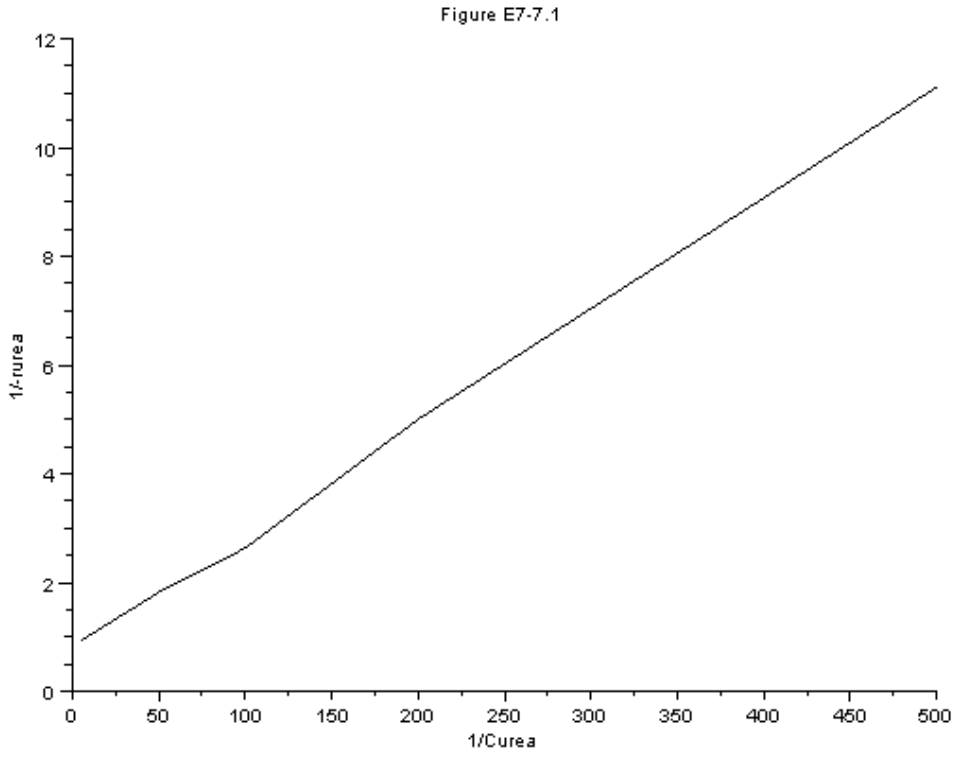

Figure 7.1: Output graph of S 7.7

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

Example 7.8 7.8data.sci

```
1  Km = 0.0266;
```

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

Example 7.8 7.8.sce

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

Example 7.9 7.9data.sci

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

Example 7.9 7.9.sce

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

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

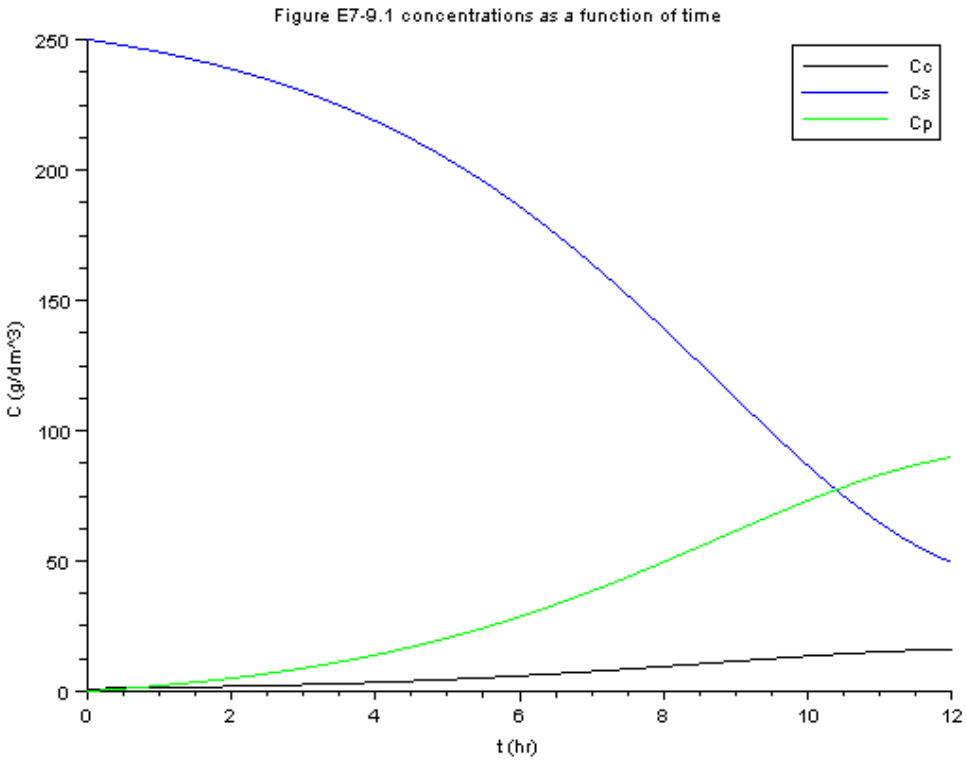

Figure 7.2: Output graph of S 7.9

Chapter 8

Steady State Nonisothermal Reactor Design

8.1 Discussion

When executing the code from the editor, use the 'Execute File into Scilab'tab and not the 'Load in Scilab'tab. The .sci files of the respective problems contain the input parameters of the question

8.2 Scilab Code

Example 8.3 8.3data.sci

```
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
```

Example 8.3 8.3.sce

```
1 clc
```

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

Example 8.4 8.4data.sci

```
T =[535 550 565 575 585 595 605 615 625]';
H0C= -226000;
H0B = -123000;
H0A = -66600;
CpC = 46;
CpB = 18;
CpA = 35;
CpM = 19.5;
TR = 528;
Ti0 = 535;
vA0 = 46.62;
vB0 = 46.62;
VM0 = 233.1;
V = 40.1;
FA0 =43.04;
FM0 = 71.87;;
FB0 = 802.8;
A = 16.96e12;
E = 32400;
R = 1.987;
```

Example 8.4 8.4.sce

```
clc
clear all
exec("8.4data.sci");
```

```
4  HRx0 = H0C-H0B-H0A;
5  deltaCp = CpC-CpB-CpA;
6  deltaHRx0 = HRx0+deltaCp*(TR-TR);
7  v0 = vA0+vB0+VM0;
8  tau = V/v0;
9  CA0 = FA0/v0;
10 phiM0 = FM0/FA0;
11 phiB0 = FB0/FA0;
12 Cpi = CpA+phiB0*CpB+phiM0*CpM;
13
14 for i =1:length(T)
15 XEB(i) = -Cpi*(T(i)-Ti0)/(deltaHRx0+deltaCp*(T(i)-TR
      ));
16 XMB(i) = tau*A*exp(-E/(R*T(i)))/(1+tau*A*exp(-E/(R*T
      (i))));
17 end
18
19
20
21 plot2d(T',[XEB XMB]);
22
23 xtitle( 'Figure E8-4.2', 'T(oR)', 'Conversion, X' )
      ;
24 legend(['XEB';'XMB']);
```

Example 8.6 8.6data.sci

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

Example 8.6 8.6.sce

```
1 clc
2 clear all
3 exec("8.6data.sci");
4  V = 0:.1:3.6;
```

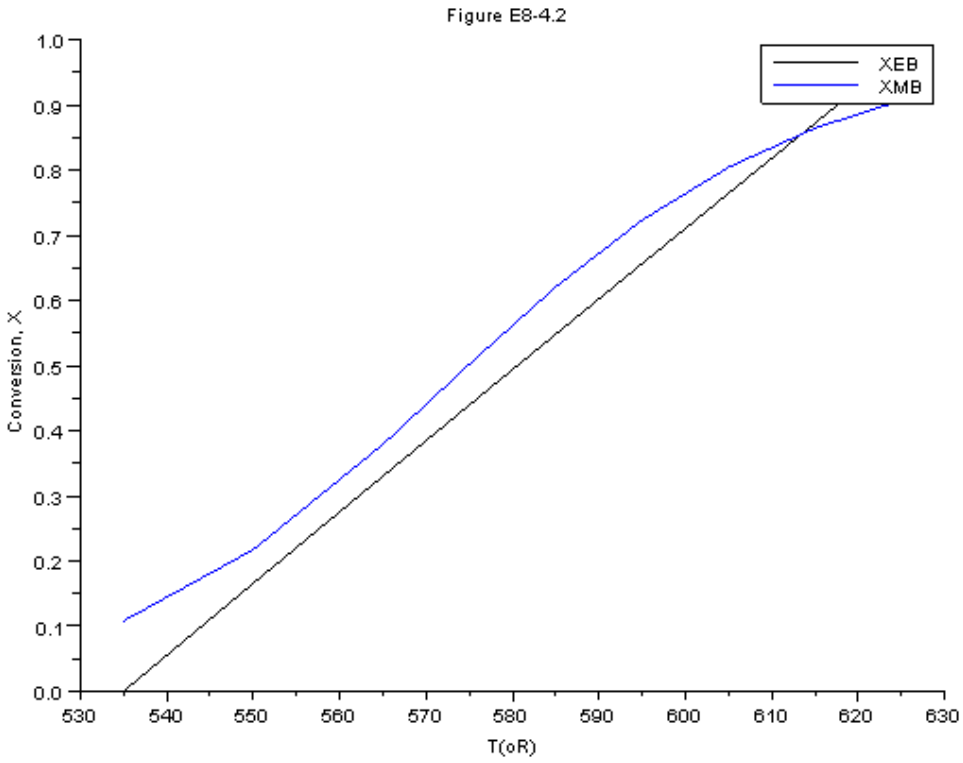

Figure 8.1: Output graph of S 8.4

```
5  function w=f(V,X)
6
7   w =zeros(1,1);
8  T =330+43.3*X;
9  k=31.1*exp(7906*(T-360)/(T*360));
10 Kc = 3.03*exp(-830.3*((T-360)/(T*360)));
11 Xe = Kc/(1+Kc);
12 ra = -k*Ca0*(1-(1+(1/Kc))*X);
13  w(1)= -ra/Fa0;
14  rate = -ra;
15 endfunction
16
17 x=ode([0],V0,V,f);
18
19 for i =1:length(x)
20   T(1,i) =330+43.3*x(1,i)
21
22   k(1,i)=31.1*exp(7906*(T(1,i)-360)/(T(1,i)*360));
23   Kc(1,i) = 3.03*exp(-830.3*((T(1,i)-360)/(T(1,i)
       *360)));
24
25   ra(1,i) = k(1,i)*Ca0*(1-(1+(1/Kc(1,i)))*x(1,i));
26 end
27 scf(1)
28 plot2d(V,x(1,:));
29
30 xtitle( 'Figure E8-6.1a', 'V(m^3)', 'X' ) ;
31 scf(2)
32 plot2d(V,T(1,:));
33
34 xtitle( 'Figure E8-6.1b', 'V(m^3)', 'T (K)' ) ;
35
36 scf(3)
37 plot2d(V,ra);
38
39 xtitle( 'Figure E8-6.1c', 'V(m^3)', '-ra (kmol/m^3hr
     )' ) ;
```

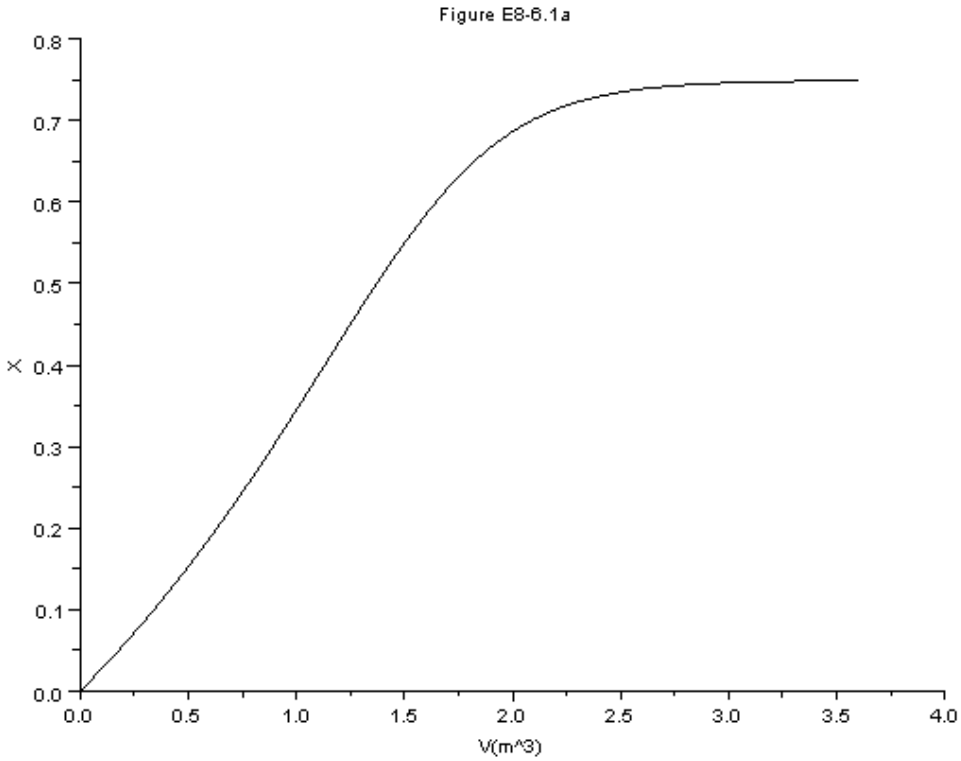

Figure 8.2: Output graph of S 8.6

Example 8.7 8.7data.sci

```
1 Fa0 =38.3;
2 Ca0 = 18.3;
3 T0 = 1035;
4 Tr = 298;
5 V0 = 0;
```

Example 8.7 8.7.sce

```
1 clc
2 clear all
```

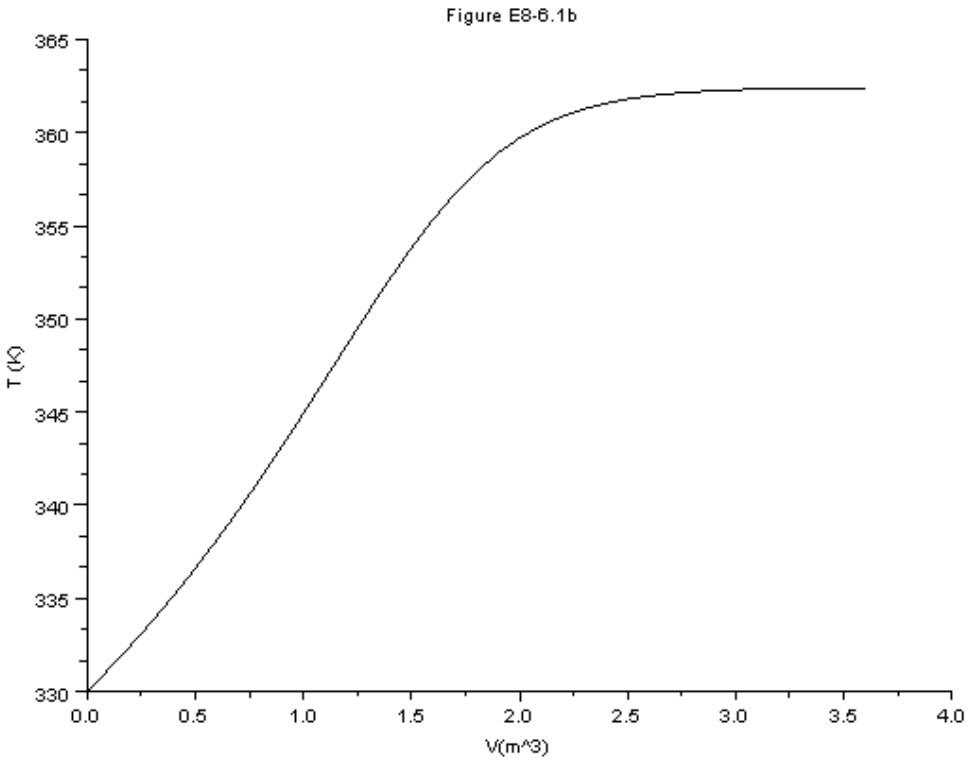

Figure 8.3: Output graph of S 8.6

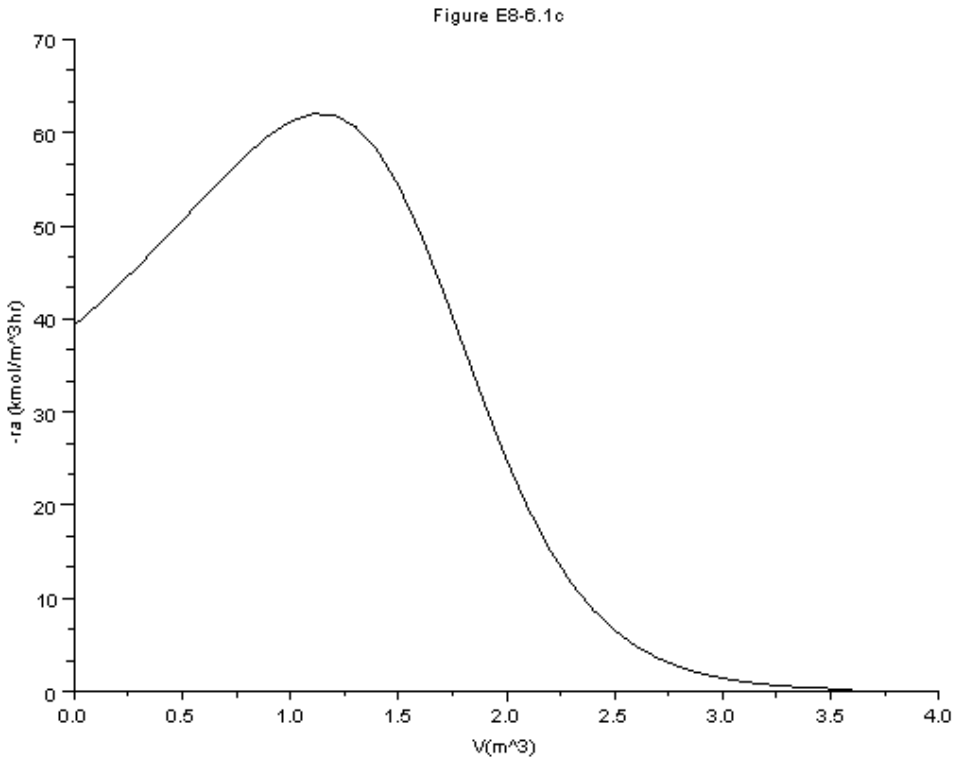

Figure 8.4: Output graph of S 8.6

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

Example 8.8 8.8data.sci

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

Example 8.8 8.8.sce

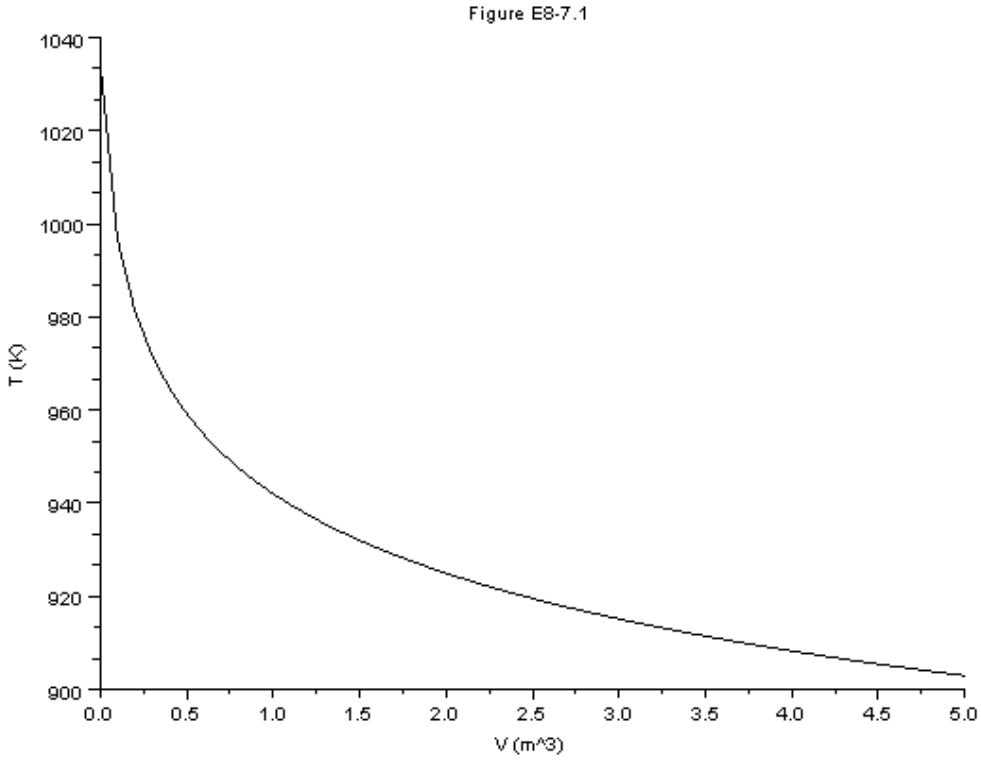

Figure 8.5: Output graph of S 8.7

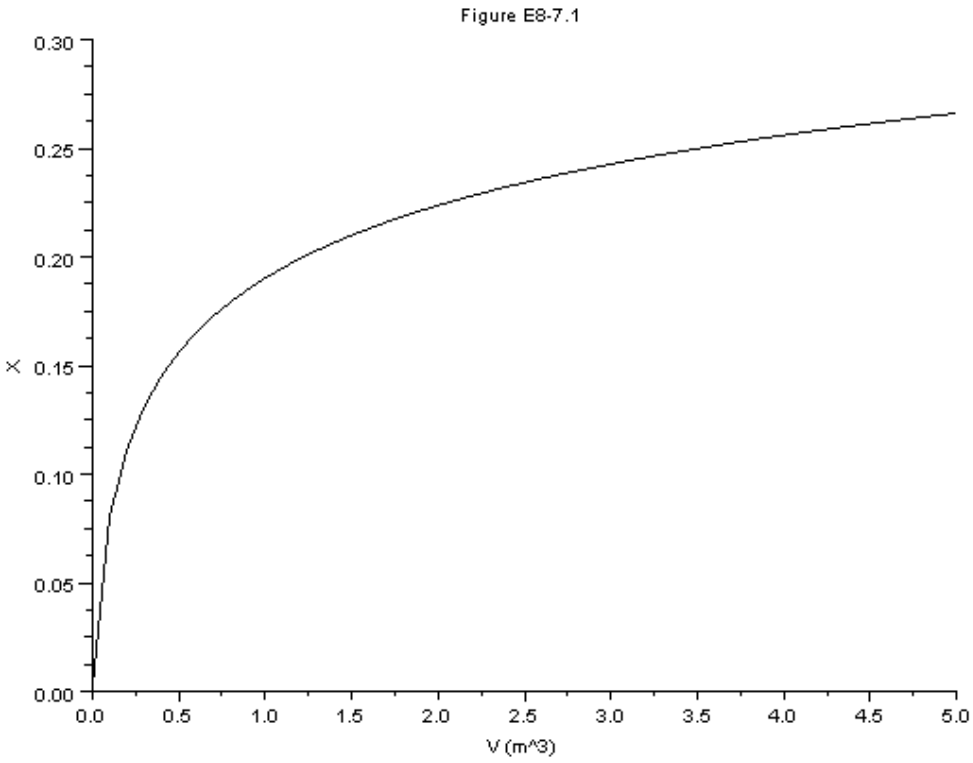

Figure 8.6: Output graph of S 8.7

```
clc
clear all
exec("8.8data.sci");
for i = 1:length(T)
  Xe(i) = 100000*exp(-33.78*(T(i)-298)/(T(i)))/(1+
     100000*exp(-33.78*(T(i)-298)/T(i)));
  XEB(i) = (2.5e-3)*(T(i)-300);
end
plot2d(T,[Xe XEB])

xtitle( 'Figure E8-8.1', 'T', 'X' ) ;
legend(['Xe';'XEB']);
```

Example 8.10 8.10.sce

```
clc
clear all
//eY(2)ec("8.6data.sci");
W = 0:1:28.58;
W0=0;
function w=f(W,Y)
  w =zeros(3,1);


fao=.188
visc=.090
Ta=1264.67
deltah=-42471-1.563*(Y(3)-1260)+.00136*(Y(3)
   **2-1260**2)-(2.459*10**(-7))*(Y(3)**3-1260**3);
summ= 57.23+.014 * Y(3)-1.94 *10**(-6.)*Y(3)**2
dcp=-1.5625+2.72*10**(-3)*Y(3)-7.38*10**(-7)*Y(3)**2
k=360D*exp(-176008/Y(3)-(110.1*log(Y(3)))+912.8)
thetaso=0;
Po=2
Pao=.22
thetao=.91
eps=-.055
```

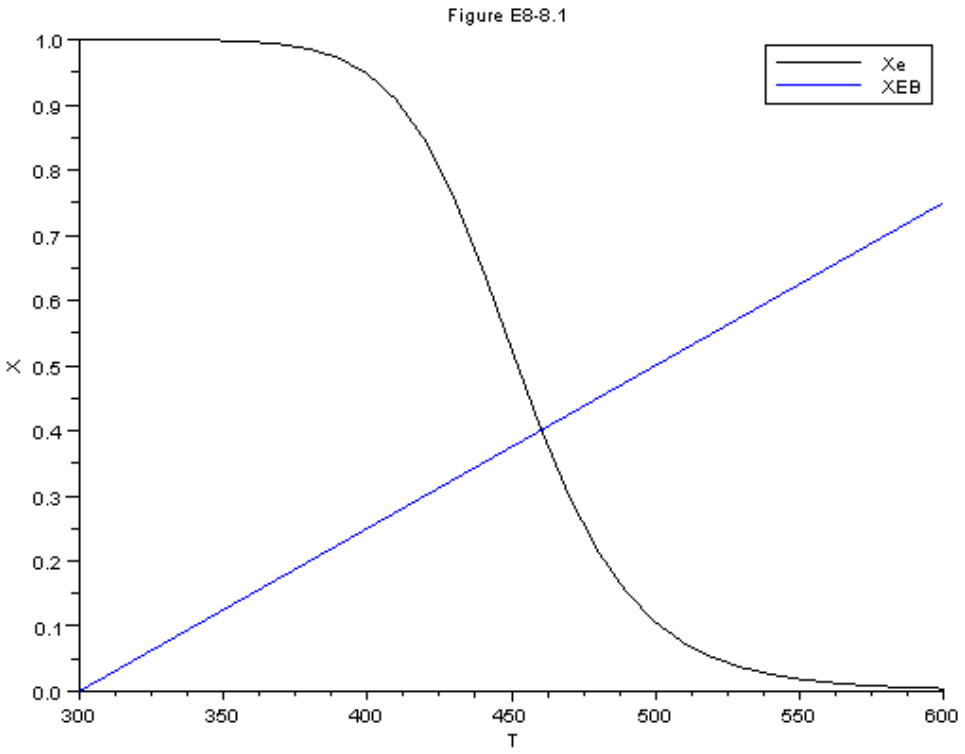

Figure 8.7: Output graph of S 8.8

```
22 R=1.987;
23 Kp=exp(42311/R/Y(3)-11.24);
24 if(Y(2)< =.05)
25
26   ra=(-k*(.848-.012/(Kp**2)));
27 else
28   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)));
29 end
30
31 w(1)=(-1.12*10**(-8)*(1-.055*Y(2))*Y(3))*(5500*visc
     +2288)/Y(1) ;
32 w(2)=-(ra)/fao ;
33 w(3)=(5.11*(Ta-Y(3))+(-ra)*(-deltah) )/(fao*(summ+Y
     (2)*dcp))
34 endfunction
35
36 X=ode([2;0;1400],W0,W,f);
37
38 plot2d(W,X(1,:));
39 plot2d(W,X(3,:));
```

Example 8.11 8.11data.sci

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

Example 8.11 8.11.sce

```
1 clc
2 clear all
3 exec("8.11data.sci");
4 V = 0:.01:1;
5
6 function w=f(V,Y)
```

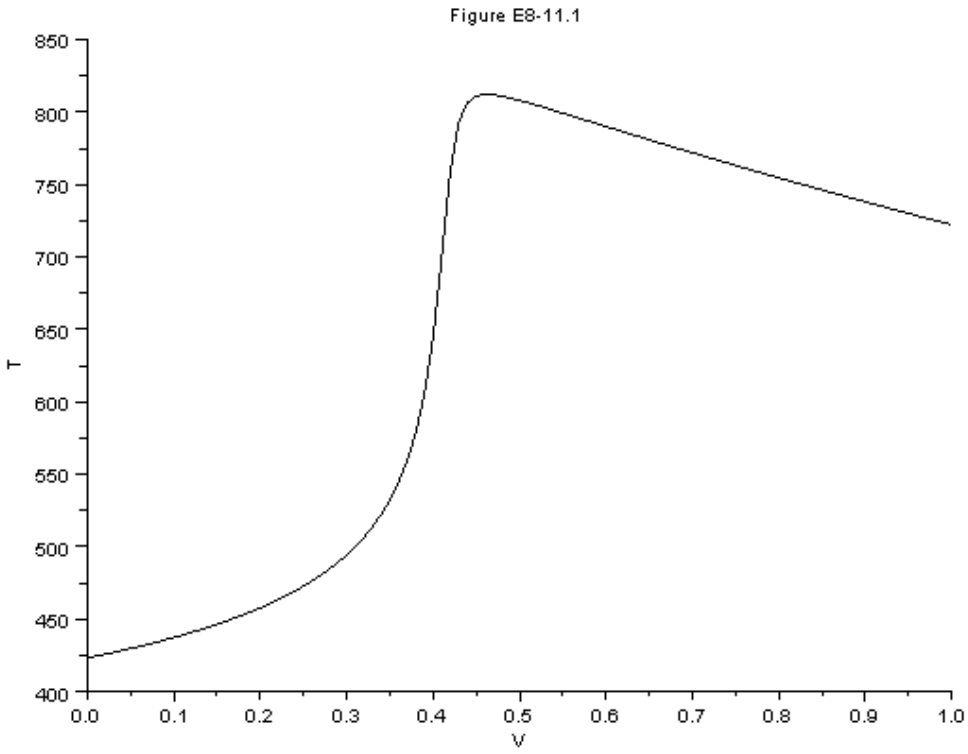

Figure 8.8: Output graph of S 8.11

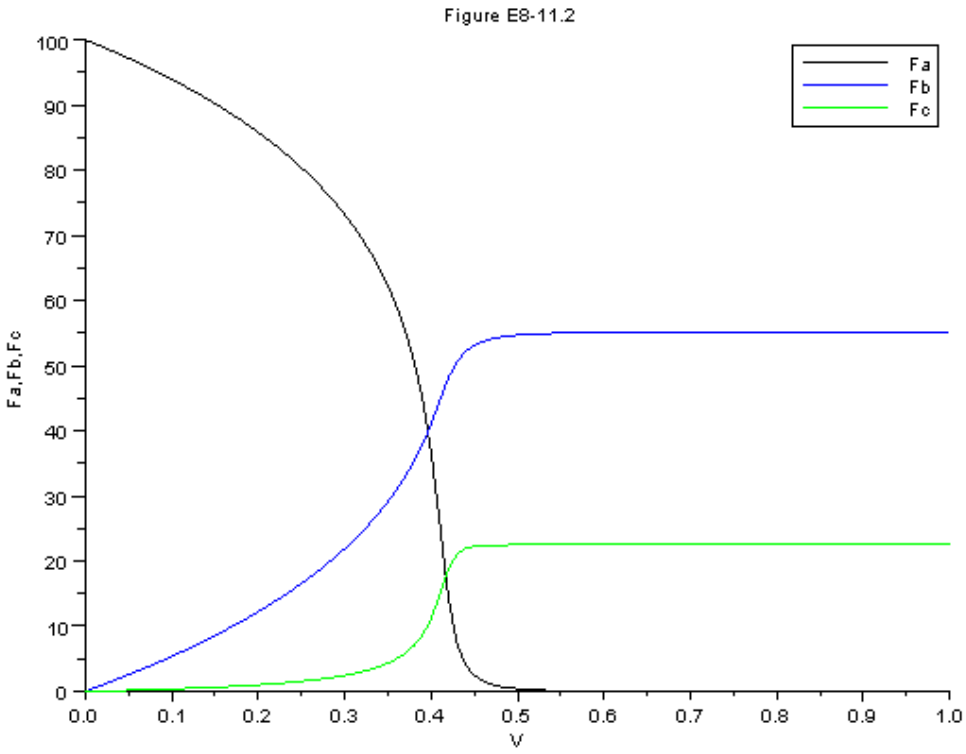

Figure 8.9: Output graph of S 8.11

```
7
8   w =zeros(4,1);
9
10  k1a=10*exp(4000*((1/300)-(1/Y(4))));
11  k2a=.09*exp(9000*((1/300)-(1/Y(4))))
12
13  Ft=Y(1)+Y(2)+Y(3);
14
15  Ca=Cto*(Y(1)/Ft)*(To/Y(4))
16  Cb=Cto*(Y(2)/Ft)*(To/Y(4))
17  Cc=Cto*(Y(3)/Ft)*(To/Y(4))
18  r1a=-k1a*Ca;
19  r2a=-k2a*Ca^2;
20
21  w(1)=r1a+r2a;
22  w(2)=-r1a;
23
24  w(3)=-r2a/2;
25  w(4)=(4000*(373-Y(4))+(-r1a)*20000+(-r2a)*60000)
       /(90*Y(1)+90*Y(2)+180*Y(3));
26  endfunction
27
28  x=ode([100;0;0;423],V0,V,f);
29
30  scf(1)
31  plot2d(V,x(4,:));
32
33  xtitle( 'Figure E8-11.1', 'V', 'T' ) ;
34
35  scf(2)
36
37  l1=x(1,: )'
38  l2=x(2,: )'
39  l3=x(3,: )'
40  plot2d(V',[l1 l2 l3]);
41
42  xtitle( 'Figure E8-11.2', 'V', 'Fa,Fb,Fc' ) ;
43  legend(['Fa';'Fb';'Fc']);
```

Example 8.12 8.12data.sci

```
Cp=200
Cao=0.3
To=283
tau=.01;
DH1=-55000;
DH2=-71500;
vo=1000;
E2=27000;
E1=9900;
UA=40000;
Ta=330;
```

Example 8.12 8.12.sce

```
clc
clear all
exec("8.12data.sci");
t=1:10:250;
for i=1:length(t)
T(i)=2*t(i)+283;

k2(i)=4.58*exp((E2/1.987)*((1/500)-(1/T(i))))
k1(i)=3.3*exp((E1/1.987)*((1/300)-(1/T(i))))
Ca(i)=Cao/(1+tau*k1(i))
kappa=UA/(vo*Cao)/Cp
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))));
Tc=(To+kappa*Ta)/(1+kappa);
Cb(i)=tau*k1(i)*Ca(i)/(1+k2(i)*tau);
R(i)=Cp*(1+kappa)*(T(i)-Tc);
Cc=Cao-Ca(i)-Cb(i);
F(i)=G(i)-R(i);
end
plot(T',[G R])
```

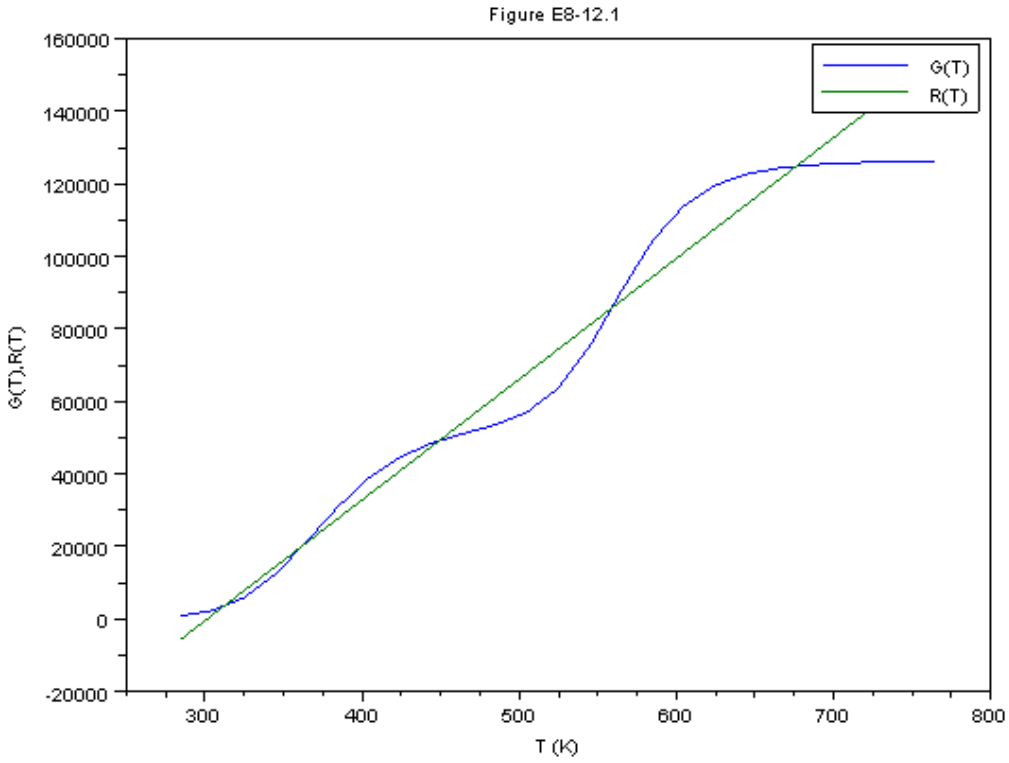

Figure 8.10: Output graph of S 8.12

```
20
21 xtitle( 'Figure E8-12.1', 'T (K)', 'G(T),R(T)' ) ;
22 legend(['G(T)';'R(T)']);
```

Chapter 9

Unsteady State Nonisothermal Reactor Design

9.1 Discussion

When executing the code from the editor, use the 'Execute File into Scilab'tab and not the 'Load in Scilab'tab. The .sci files of the respective problems contain the input parameters of the question

9.2 Scilab Code

Example 9.1 9.1data.sci

```
1 t0=0;
```

Example 9.1 9.1.sce

```
1 clc
2 clear all
3 exec("9.1data.sci");
4  t = 0:10:1500;
5 function w=f(t,x)
6
7  w =zeros(1,1);
```

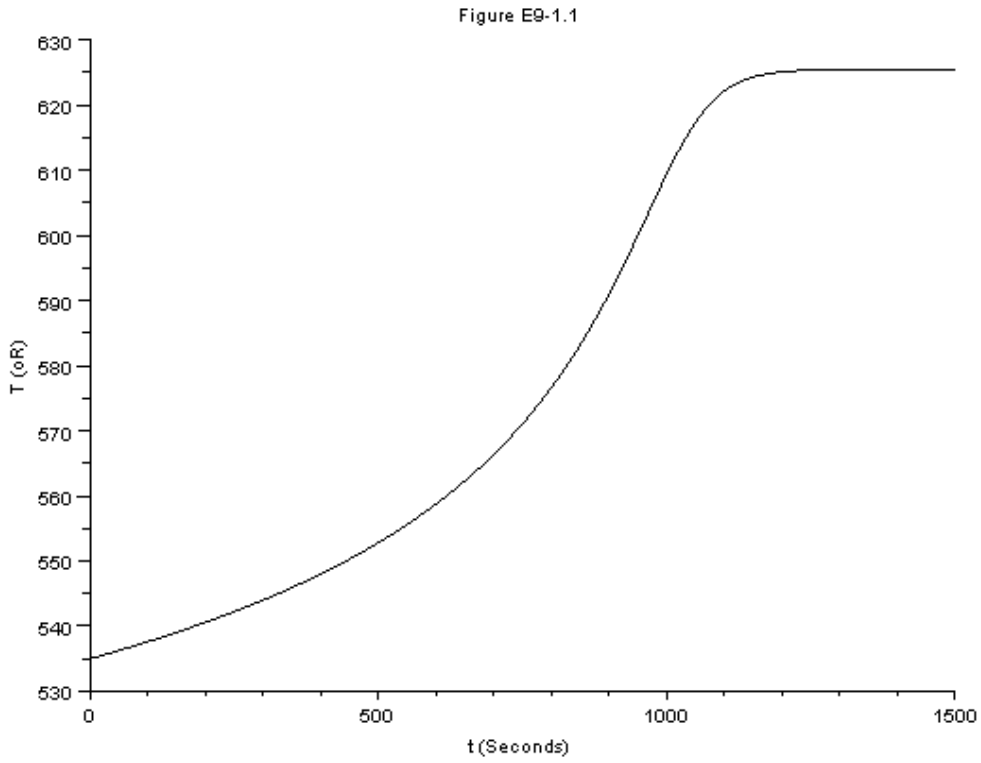

Figure 9.1: Output graph of S 9.1

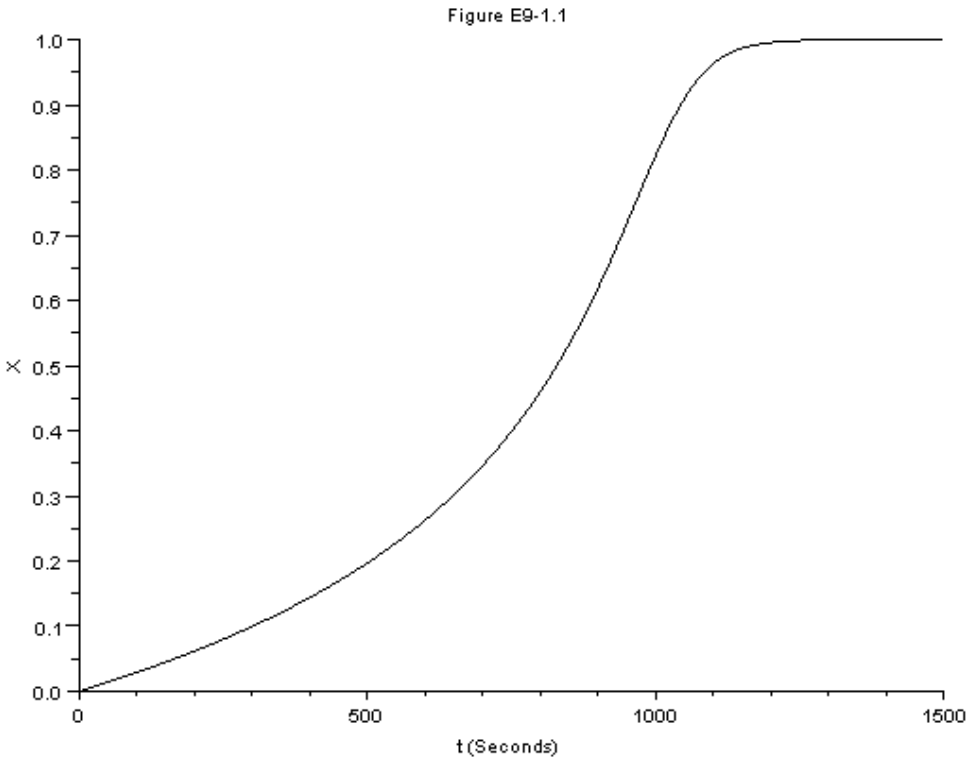

Figure 9.2: Output graph of S 9.1

```
8
9  t1=535+90.45*x
10 k= .000273*exp(16306*((1/535)-(1/t1)));
11 w(1)=k*(1-x)
12 endfunction
13
14 X=ode([0],t0,t,f);
15 T=535+90.45*X;
16 scf(1)
17 plot2d(t,T);
18
19 xtitle( 'Figure E9-1.1', 't (Seconds)', 'T (oR)' ) ;
20
21 scf(2)
22 plot2d(t,X);
23
24 xtitle( 'Figure E9-1.1', 't (Seconds)', 'X' ) ;
```

Example 9.2 9.2data.sci

```
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;
```

Example 9.2 9.2.sce

```
1 clc
2 clear all
3 //this code is only for Part C
4 exec("9.2data.sci");
5  t = 55:1:121;
6 function w=f(t,Y)
7
```

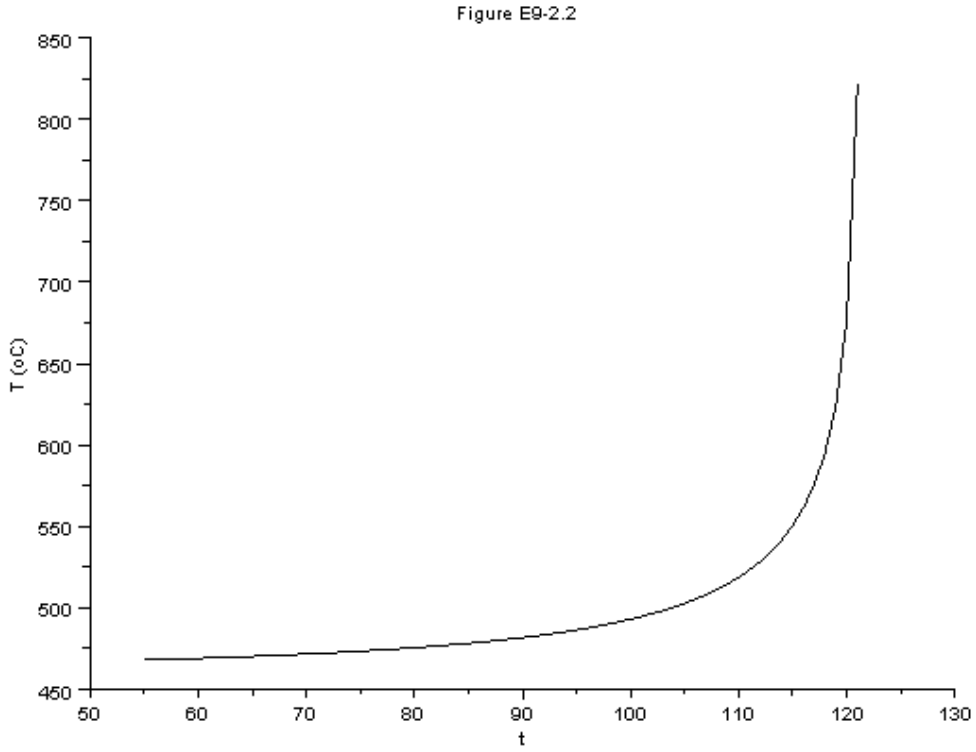

Figure 9.3: Output graph of S 9.2

```
 w =zeros(2,1);


k=.00017*exp(11273/(1.987)*(1/461-1/Y(1)))
Qr=UA*(Y(1) -298)
Theata=Nbo/Nao
ra=-k*(Nao**2)*(1-Y(2))*(Theata-2*Y(2))/(U**2)
rate=-ra
Qg=ra*U*(dH)
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)' ) ;
```

Example 9.3 9.3data.sci

```
v0=.004;
Cb0=1;
UA=3000;
Ta=290;
cp=75240;
T0=300;
dh=-7.9076e7;
Cw0=55;
cpa=170700;
Vi=.2;
t0=0;
```

Example 9.3 9.3.sce

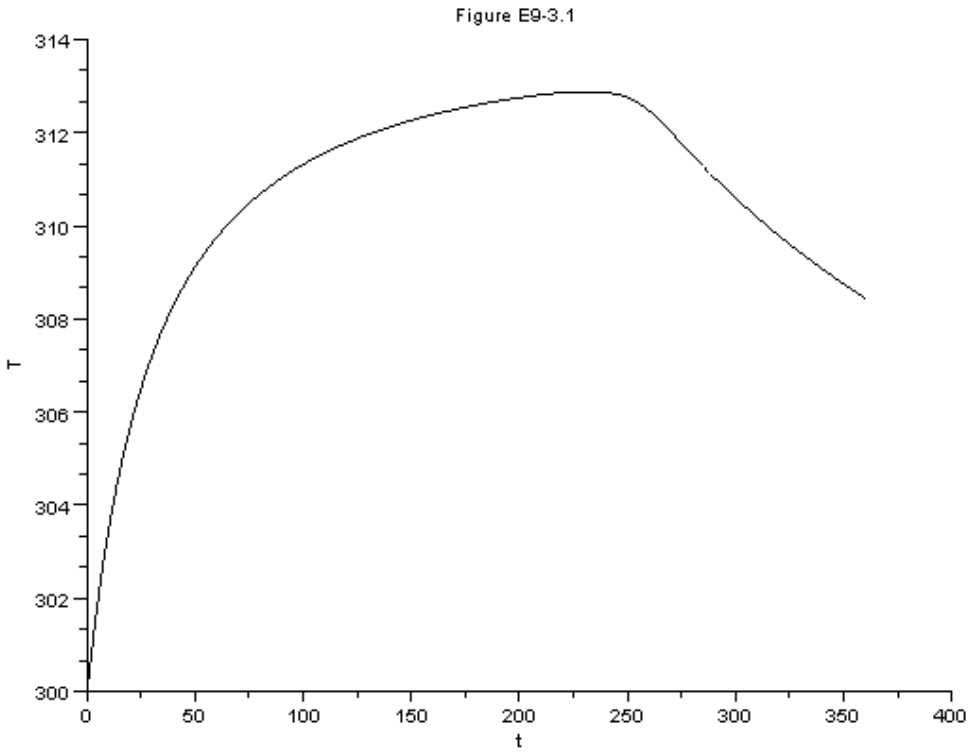

Figure 9.4: Output graph of S 9.3

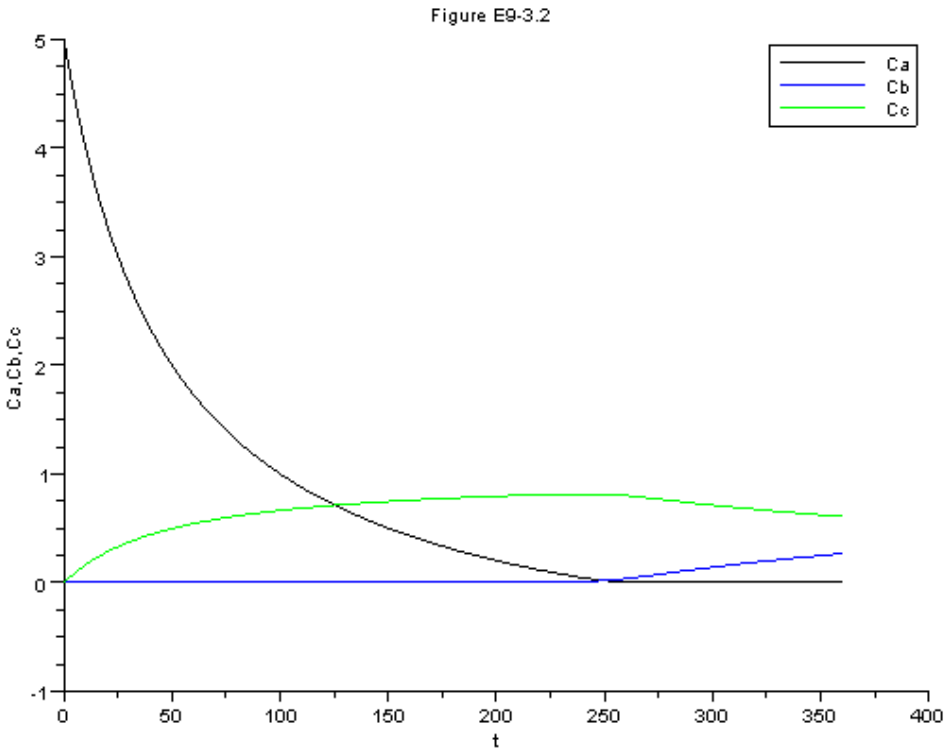

Figure 9.5: Output graph of S 9.3

```
clc
clear all
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' ) ;

```

```
38 scf(2)
39 l1=x(1,: )'
40 l2=x(2,: )'
41 l3=x(3,: )'
42 plot2d(t',[l1 l2 l3]);
43
44 xtitle( 'Figure E9-3.2', 't', 'Ca,Cb,Cc' ) ;
45 legend(['Ca';'Cb';'Cc']);
```

Example 9.4 9.4data.sci

```
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;
```

Example 9.4 9.4.sce

```
1 clc
2 clear all
3 //exec("9.3data.sci");
4 t = 0:.0001:4;
5 t0=0;
6 function w=f(t,Y)
7
8  w =zeros(5,1);
9
10 Fa0=80;
11 T0=75;
12 V=(1/7.484)*500;
13 UA=16000;
14 Ta1=60;
15 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;
endfunction

x=ode([0;3.45;0;0;75],t0,t,f);
scf(1)
plot2d(t,x(1,:));

xtitle( 'Figure E9-4.1', 't', 'Ca' ) ;

scf(2)
plot2d(t,x(5,:));

xtitle( 'Figure E9-4.2', 't', 'T' ) ;
scf(3)
plot2d(x(5,:),x(1,:));
```

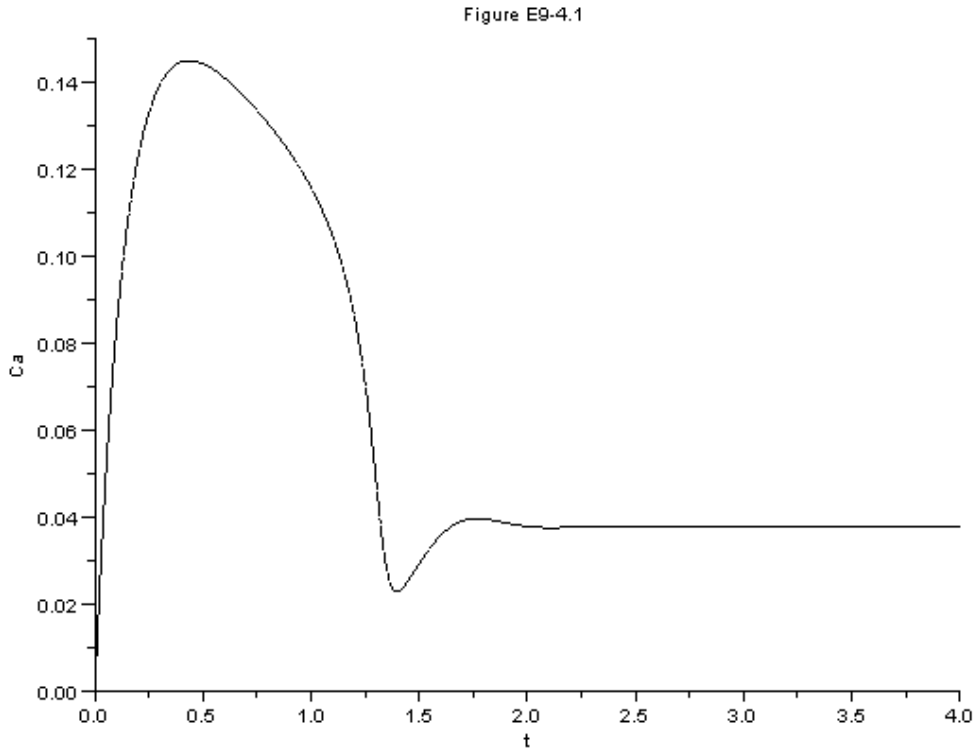

Figure 9.6: Output graph of S 9.4

```
54
55 xtitle( 'Figure E9-4.3', 'T', 'Ca' ) ;
```

Example 9.8 9.8data.sci

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

Example 9.8 9.8.sce

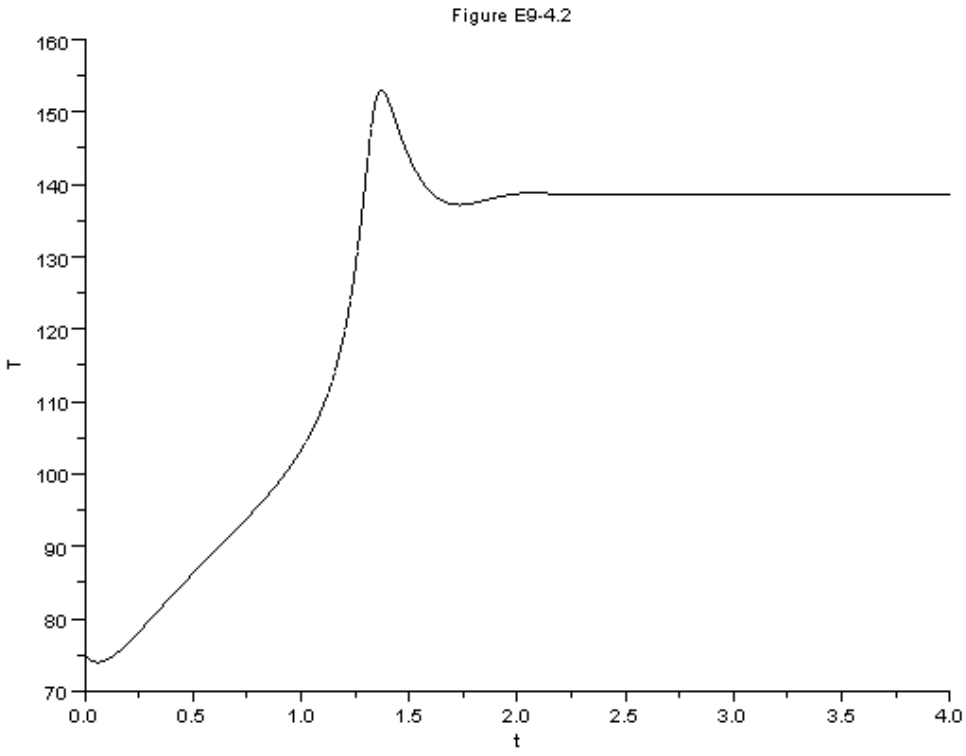

Figure 9.7: Output graph of S 9.4

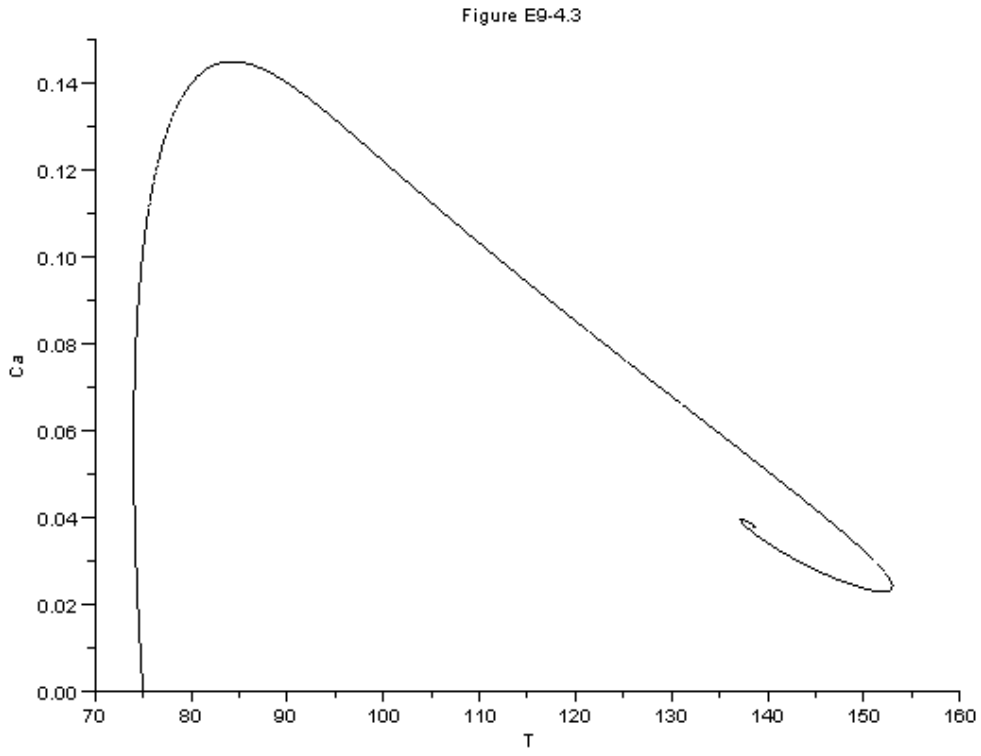

Figure 9.8: Output graph of S 9.4

```
clc
clear all
exec("9.8data.sci");
t = 0:.01:1.5;

function w=f(t,Y)

 w =zeros(4,1);

k1a=1.25*exp((9500/1.987)*((1/320)-(1/Y(4))));
k2b=0.08*exp((7000/1.987)*((1/290)-(1/Y(4))));
ra=-k1a*Y(1);
V=100+vo*t;
rc=3*k2b*Y(2);
rb=k1a*(Y(1)/2)-k2b*Y(2);
w(1)=ra+(Cao-Y(1))*vo/V;
w(2)=rb-Y(2)*vo/V;
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);
endfunction

x=ode([1;0;0;290],t0,t,f);


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

xtitle( 'Figure E9-8.1', 't', 'Ca,Cb,Cc' ) ;
legend(['Ca';'Cb';'Cc']);

scf(2)
plot2d(t,x(4,:));

xtitle( 'Figure E9-8.2', 't', 'T' ) ;
```

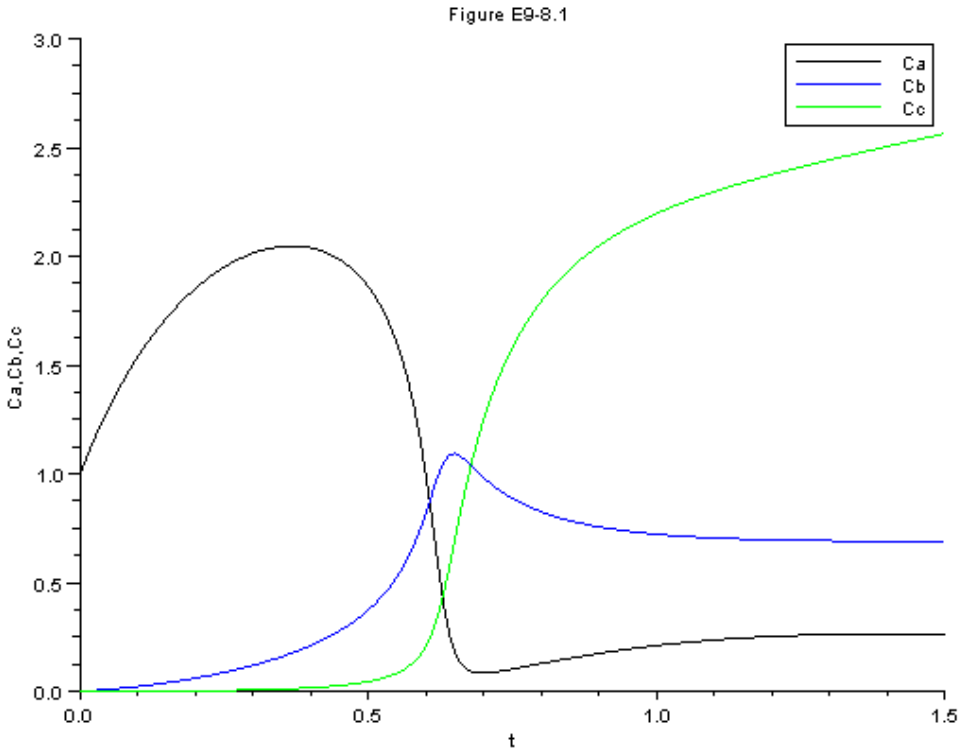

Figure 9.9: Output graph of S 9.8

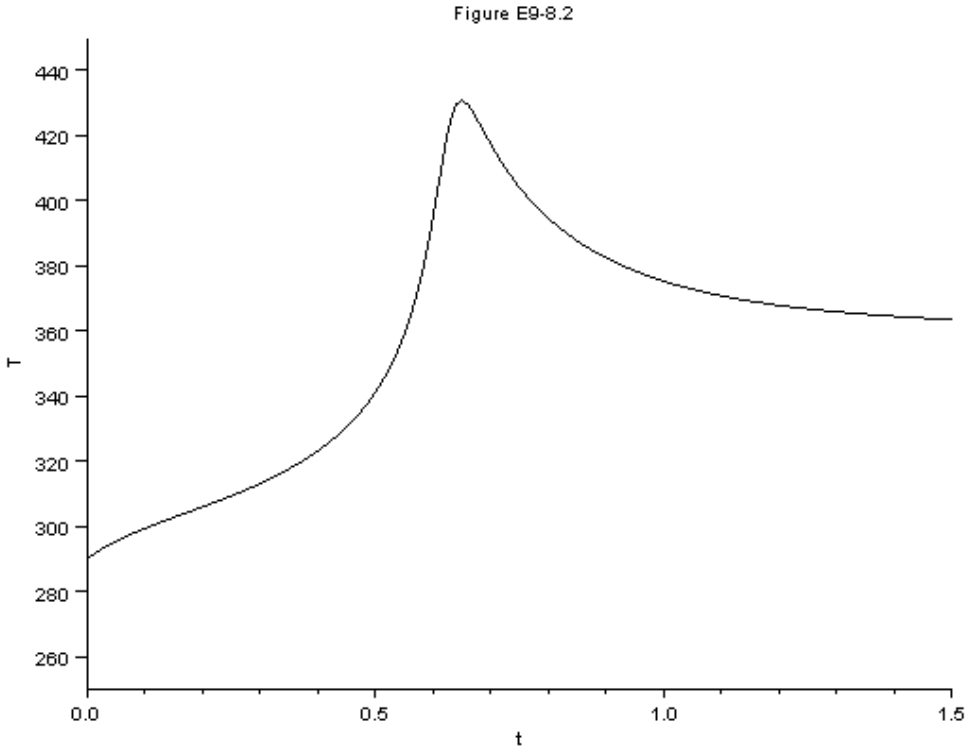

Figure 9.10: Output graph of S 9.8

Chapter 10

Catalysis and Catalytic Reactors

10.1 Discussion

When executing the code from the editor, use the 'Execute File into Scilab'tab and not the 'Load in Scilab'tab. The .sci files of the respective problems contain the input parameters of the question

10.2 Scilab Code

Example 10.3 10.3data.sci

```
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;
```

Example 10.3 10.3.sce

```
1 clc
2 clear all
```

```
exec("10.3data.sci");
w = 0:10:10000;

function W=f(w,x)

 W =zeros(1,1);

pt0=.3*Po;
y=(1-alpha*w)^.5;
ph=pt0*(1.5-x)*y;
pt=pt0*(1-x)*y;
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'
```

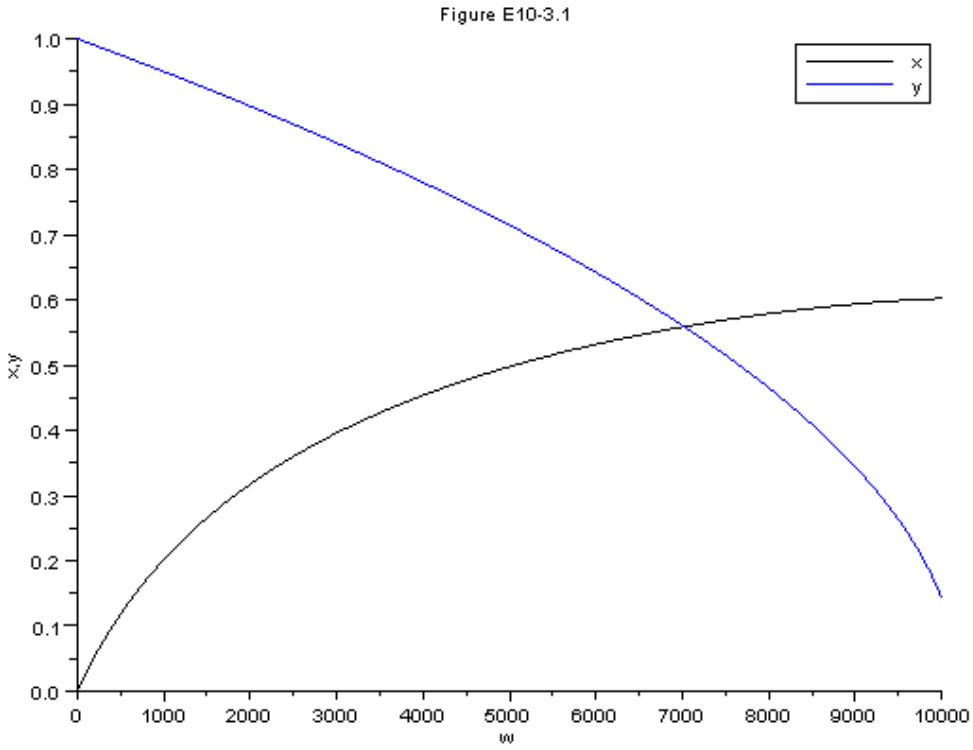

Figure 10.1: Output graph of S 10.5

```
41 l3=pb'
42 plot2d(w',[l1 l2 l3]);
43
44 xtitle( 'Figure E10-3.2', 'w', 'ph,pt,pb' ) ;
45 legend(['ph';'pt';'pb']);
```

Example 10.5 10.5data.sci

```
1 kd=9;
2 Ca0=.8;
3 tau=.02
```

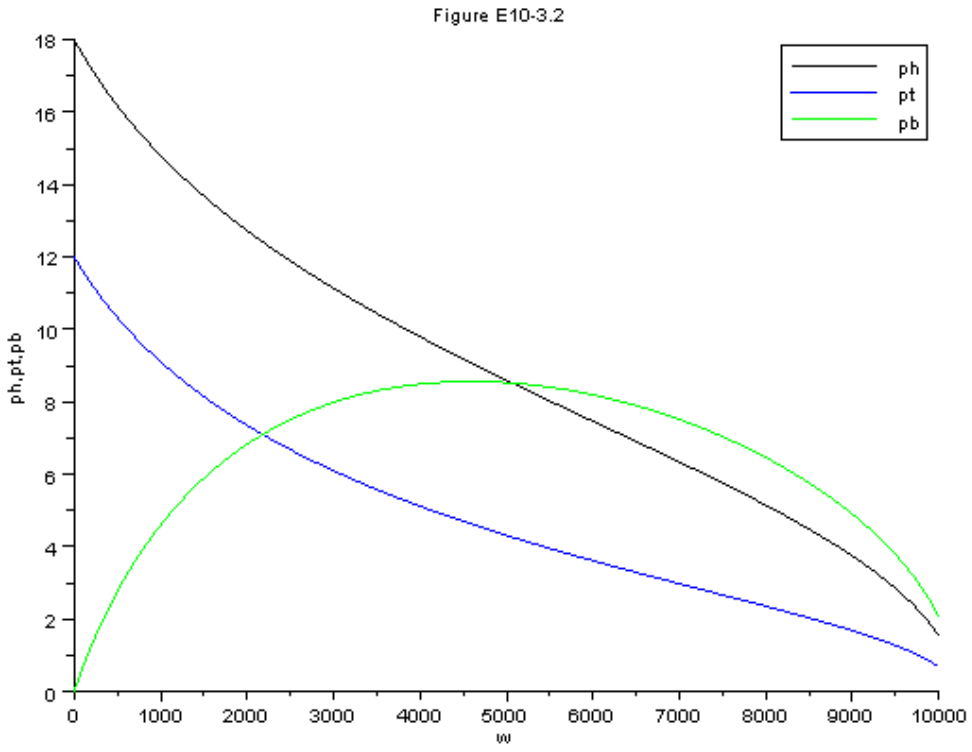

Figure 10.2: Output graph of S 10.5

```
k=45;
Ct0=1;
t0=0
```

Example 10.5 10.5.sce

```
clc
clear all
exec("10.5data.sci");
t = 0:.01:.5;

function w=f(t,Y)

 w =zeros(2,1);


ya0=Ca0/Ct0;
X=1-(1+ya0)/(1+Y(2)/Ct0)*Y(2)/Ca0;
w(1)=-kd*Y(1)*Y(2);
w(2) = (Ca0/tau)-((1+ya0)/(1+(Y(2)/Ct0))+tau*Y(1)*k)
   *Y(2)/tau;
endfunction

x=ode([1;.8],t0,t,f);
Ca0=.8;
Ct0=1
ya0=Ca0/Ct0;
for i=1:length(t)
  X1(i)=1-(1+ya0)/(1+x(2,i)/Ct0)*x(2,i)/Ca0;
  end


l1=x(1,:)'
l2=x(2,:)'
l3=X1;
plot2d(t',[l1 l2 l3]);

xtitle( 'Figure E10-5.1', 't', 'a,Ca,X' ) ;
```

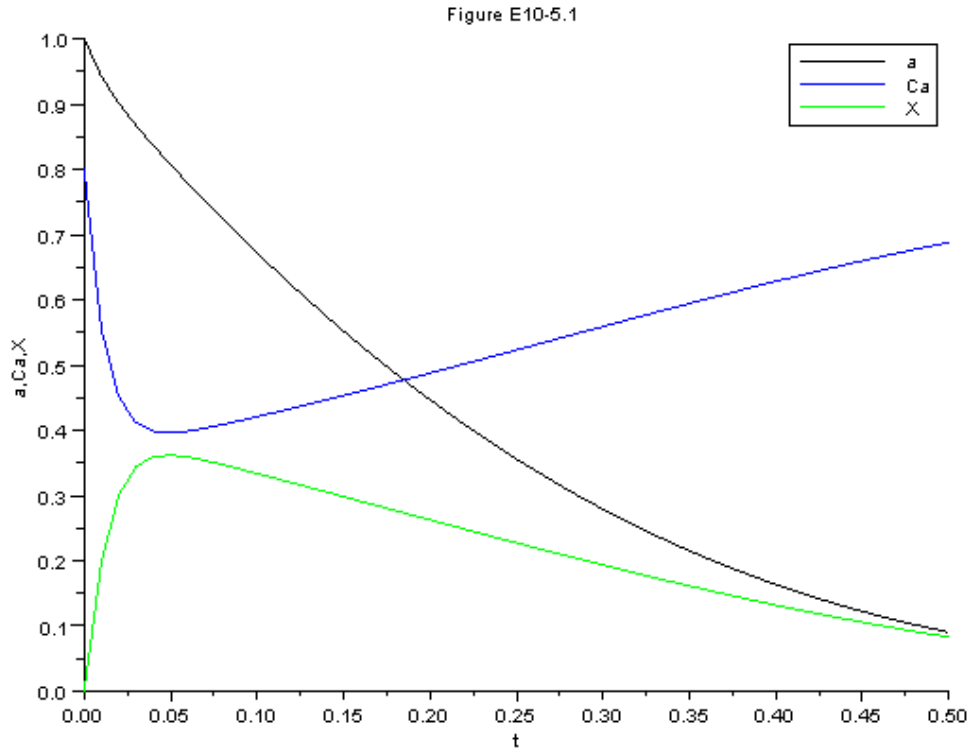

Figure 10.3: Output graph of S 10.5

```
32 legend(['a';'Ca';'X']);
```

Example 10.7 10.7data.sci

```
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;
```

```
Kc=.1;
rho=80;
kprime=0.0014;
D=1.5;
Uo=2.5;
```

Example 10.7 10.7.sce

```
clc
clear all
exec("10.7data.sci");
z = 0:.1:10;
z0=0;
function w=f(z,X)

 w =zeros(1,1);


U=Uo*(1+eps*X)
Pa=Pao*(1-X)/(1+eps*X)
Pb=Pao*X/(1+eps*X)
vo=Uo*3.1416*D*D/4
Ca0=Pao/R/T
Kca=Ka*R*T
Pc=Pb
a=1/(1+A*(z/U)**0.5)
raprime=a*(-kprime*Pa/(1+ Ka*Pa+Kb*Pb+Kc*Pc))
ra=rho*raprime;
w(1)=-ra/U/Ca0
endfunction

x=ode([0],z0,z,f);
for i=1:length(z)
U(1,i)=Uo*(1+eps*x(1,i))
a(1,i)=1/(1+A*(z(1,i)/U(1,i))**0.5)
end


```

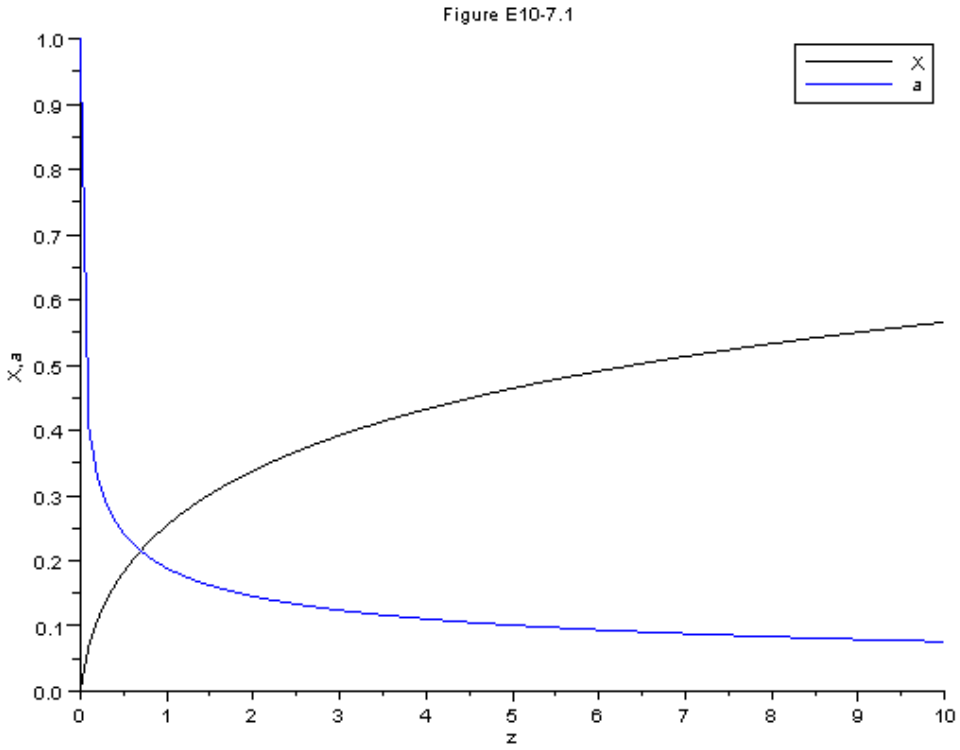

Figure 10.4: Output graph of S 10.7

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

Chapter 11

External Diffusion Effects on Hetrogeneous Reactions

11.1 Discussion

When executing the code from the editor, use the 'Execute File into Scilab'tab and not the 'Load in Scilab'tab. The .sci files of the respective problems contain the input parameters of the question

11.2 Scilab Code

Example 11.1 11.1data.sci

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

Example 11.1 11.1.sce

```
1 clc
2 clear all
3 exec("11.1data.sci");
```

```
4 WAZ1=DAB*CT0*(yAb-yAs)/s;
5 WAZ2=c*DAB*CT0*log((1-yAs)/(1-yAb))/s;
6 disp(WAZ1)
7 disp(WAZ2)
```

Example 11.3 11.3data.sci

```
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
```

Example 11.3 11.3.sce

```
1  clc
2  clear all
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;
```

```
Shprime=((Reprime)^.5)*Sc^(1/3);
kc=DAB*(1-phi)*Y*(Shprime)/(dp*phi);
X=1-exp(-kc*ac*z/U);
disp("X =")
disp(X)
```

Example 11.4 11.4data.sci

```
X1=.865;
```

Example 11.4 11.4.sce

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

Example 11.5 11.5data.sci

```
X1=.865;
T1=673;
T2=773;
```

Example 11.5 11.5.sce

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

Chapter 12

Diffusion and Reaction in Pours Catalysts

12.1 Discussion

When executing the code from the editor, use the 'Execute File into Scilab'tab and not the 'Load in Scilab'tab. The .sci files of the respective problems contain the input parameters of the question

12.2 Scilab Code

Chapter 13

Distributions of Residence Times for Chemical Reactions

13.1 Discussion

When executing the code from the editor, use the 'Execute File into Scilab'tab and not the 'Load in Scilab'tab. The .sci files of the respective problems contain the input parameters of the question

13.2 Scilab Code

Example 13.8 13.8data.sci

```
1 k=0.01
2 cao=8;
3 z0=0;
```

Example 13.8 13.8.sce

```
1 clc
2 clear all
3 exec("13.8data.sci");
4 z = 0:1:200;
5
6 function w=f(z,x)
```

```
7
8   w =zeros(1,1);
9
10  lam=200-z;
11  ca=cao*(1-x)
12  E1=4.44658e-10*(lam^4)-1.1802e-7*(lam^3)+1.35358e
       -5*(lam^2)-.00086
13  5652*lam+.028004;
14  E2=-2.64e-9*(lam^3)+1.3618e-6*(lam^2)-.00024069*lam
       +.015011
15  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;
16  F2=-(-9.3076e-8*lam^3+5.02846e-5*lam^2-.00941*lam
       +.61823-1)
17  ra=-k*ca^2;
18  if lam< =70
19    E=E1
20  else
21    E=(E2)
22    end
23    if(lam< =70)
24      F=F1
25    else
26      F=F2
27      end
28      EF=E/(1-F)
29      w(1)=-(ra/cao+E/(1-F)*x)
30  endfunction
31
32  X=ode([0],z0,z,f);
33
34  plot2d(z,X);
```

Example 13.9 13.9data.sci

```
1  k1=1;
2  k2=1;
3  k3=1;
```

```
t0=0;
```

Example 13.9 13.8.sce

```
clc
clear all
exec("13.9data.sci");
t = 0:.1:2.52;

function w=f(t,Y)

 w =zeros(10,1);

E1=-2.104*t^4+4.167*t^3-1.596*t^2+0.353*t-.004
E2=-2.104*t^4+17.037*t^3-50.247*t^2+62.964*t-27.402
rc=k1*Y(1)*Y(2)
re=k3*Y(2)*Y(4)
ra=-k1*Y(1)*Y(2)-k2*Y(1)
rb=-k1*Y(1)*Y(2)-k3*Y(2)*Y(4)
if t< =1.26
  E=E1
else
  E=E2
  end
  rd=k2*Y(1)-k3*Y(2)*Y(4)

  w(1)=ra
w(2) =rb
w(3) =rc
w(6)=Y(1)*E
w(7)=Y(2)*E
w(8)=Y(3)*E
w(4)=rd
w(5) =re
w(9)=Y(4)*E
w(10)=Y(5)*E
endfunction

```

```
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

14.1 Discussion

When executing the code from the editor, use the 'Execute File into Scilab'tab and not the 'Load in Scilab'tab. The .sci files of the respective problems contain the input parameters of the question

14.2 Scilab Code

Example 14.3 14.3.sce

```
1  clc
2  clear all
3
4  t = 0:10:200;
5
6  function w=f(t,Y)
7
8   w =zeros(2,1);
9
10 CTe1=2000-59.6*t+.64*t^2-0.00146*t^3-1.047*10^(-5)*t
      ^4
11 Beta=.1
12 CTe2=921-17.3*t+.129*t^2-0.000438*t^3+5.6*10^(-7)*t
      ^4
```

```
13 alpha=.8
14 tau=40
15 if(t<80)
16   CTe=CTe1
17 else
18   CTe=CTe2
19 end
20
21 w(1)=(Beta*Y(2)-(1+Beta)*Y(1))/alpha/tau
22 w(2)=(Beta*Y(1)-Beta*Y(2))/(1-alpha)/tau
23 endfunction
24
25 X=ode([2000;0],t0,t,f);
26
27 t=t';
28 for i =1:length(t)
29 CTe1(i)=2000-59.6*t(i)+.64*(t(i)^2)-0.00146*(t(i)^3)
      -1.047*(10^(-5))*t(i)^4;
30 CTe2(i)=921-17.3*t(i)+.129*t(i)^2-0.000438*t(i)
      ^3+5.6*10^(-7)*t(i)^4
31 if(t(i)<80)
32   CTe(i)=CTe1(i)
33 else
34   CTe(i)=CTe2(i)
35 end
36 end
37
38
39 l1=X(1,: )';
40 l2=CTe;
41
42 plot2d(t,[l1 l2]);
43
44 xtitle( 'Figure E14-3.1', 't', 'CT1,CTe' ) ;
45 legend(['CT1';'CTe']);
```

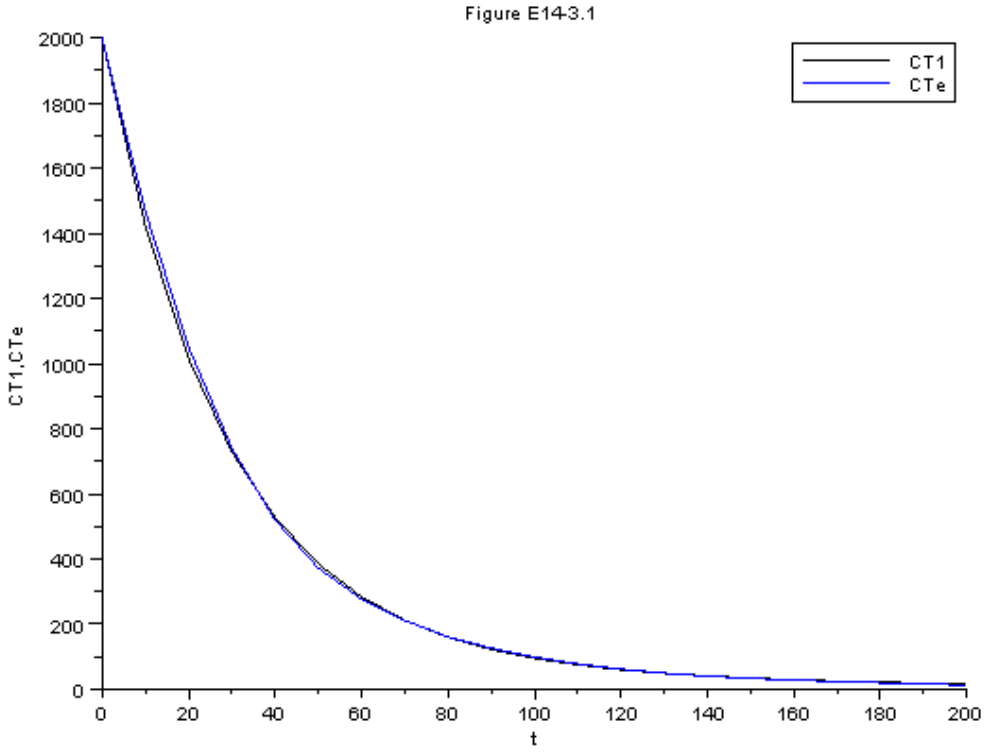

Figure 14.1: Output graph of S 14.3