

Scilab Textbook Companion for
Chemical Reaction Engineering
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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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Chapter 1

Overview of Chemical Reaction Engineering

Scilab code Exa 1.1 The Rocket Engine

```
1 clear
2 clc
3 //l=75 cm,d=60 cm,H2O Produced=108kg/s
4 l=0.75;d=0.6;
5 V=(3.14*d*d*l)/4;
6 //H2+0.5*O2=H2O
7 //Molecular wt of H2O=18
8 M=18;
9 //H2O Produced in kmol/s
10 H2O_produced=108/M;
11 //H2 used
12 H2_used=H2O_produced;
13 //O2 Used
14 O2_used=0.5*H2O_produced;
15 //Rate of reaction
16 //Rate of reaction of H2(mol/m^3.s)
17 r_H2=(H2_used/V)*1000;
18 //Rate of reaction of O2(mol/m^3.s)
19 r_O2=(O2_used/V)*1000;
```

```
20 printf("\nRESULT\n")
21 printf("rate of reaction of H2(mol/m^3.s) is %f\n",
    r_H2)
22 printf("\nrate of reaction of O2(mol/m^3.s) is %f\n"
    ,r_O2)
```

Scilab code Exa 1.2 The Living Person

```
1 clear
2 clc
3 // Assuming density of a person=1000kg/m3
4 d=1000;
5 mass=75;
6 V=mass/d;
7 //moles of O2 consumed per day
8 O2_used=(6000/2816)*6;
9 // Rate of reaction (mol/m3.s)
10 r_O2=(O2_used/V)/(24*3600);
11 printf("\nRESULT\n")
12 printf("rate of reaction of O2(mol/m^3.s) is %f\n",
    r_O2)
```

Chapter 2

Kinetics of Homogeneous Reactions

Scilab code Exa 2.1 Search for the reaction mechanism

```
1 clear
2 clc
3 //Theoretical Questions
4 printf("Its a theoretical Question")
```

Scilab code Exa 2.2 Search for a mechanism for the enzyme substrate reaction

```
1 clear
2 clc
3 //Theoretical Questions
4 printf("Its a theoretical Question")
```

Scilab code Exa 2.3 Search for the activation energy of a pasteurization process

```
1 clear
2 clc
3 // Given
4 //t1=30 min ;T1=336 k;
5 //t2=15 sec ;T2=347 k;
6 // Converting t2 in min
7 t1=30;T1=336;t2=0.25;T2=347
8 R=8.314;
9 //log(t1/t2)=E(1/T1-1/T2)/R
10 E=(log(t1/t2)*R)/(1/T1-1/T2);
11 printf("\nRESULT\n")
12 printf("E(J/mol) is %f",E)
```

Chapter 3

Interpretation of Batch Reactor Data

Scilab code Exa 3.1 Find a rate equation using the integral method

```
1 clear
2 clc
3 //Given
4 t=[0 20 40 60 120 180 300];
5 C_A=[10 8 6 5 3 2 1];
6 CAo=10;
7 //Guessing 1st order kinetics
8 //This means log(CAo/C_A) vs t should give a
   straight line
9 for i=1:7
10     k(i)=log(CAo/C_A(i));
11     CA_inv(i)=1/C_A(i);
12 end
13 //plot(t,k)
14 //This doesn't give straight line.
15 //Guessing 2nd Order Kinetics so
16 //1/C_A vs t should give a straight line
17 //plot(t,CA_inv)
18 //Again this doesn't give a straight line
```

```

19 //Guessing nth order kinetics and using fractional
    life method with F=80%
20 //log Tf=log(0.8^(1-n)-1/(k(n-1)))+(1-n)logCAo
21 //plot(t,CA)
22
23 //Picking different values of CAo
24 //Time needed for 3 runs,,from graph
25 T=[18.5;23;35];
26 CAo=[10;5;2];
27 for i=1:3
28     CA(i)=0.8*CAo(i);
29     log_Tf(i)=log10(T(i));
30     log_CAo(i)=log10(CAo(i));
31 end
32 plot(log_CAo,log_Tf)
33 xlabel('log CAo');ylabel('log t');
34 coeff1=regress(log_CAo,log_Tf);
35 n=1-coeff1(2);
36 printf("From graph we get slope and intercept for
    calculating rate eqn")
37 k1=((0.8^(1-n))-1)*(10^(1-n))/(18.5*(n-1));
38 printf("\n The rate equation is given by %f",k1)
39 printf("CA^1.4 mol/litre.sec")

```

Scilab code Exa 3.2 Find a rate equation to fit a set of data using the differential method

```

1 clear
2 clc
3 CA=[10;8;6;5;3;2;1]; //mol/litre
4 T=[0;20;40;60;120;180;300]; //sec
5 //plot(T,CA)
6 //xlabel('Time(sec)');ylabel('CA(mol/litre)');
7 //From graph y=-dCA/dt at different points are
8 y

```

```

    =[-0.1333;-0.1031;-0.0658;-0.0410;-0.0238;-0.0108;-0.0065];

9 //Guessing nth rate order
10 //rA=kCA^n
11 //log(-dCA/dt)=logk+nlogCA
12 for i=1:7
13 log_y(i)=log10(y(i));
14 log_CA(i)=log10(CA(i));
15 end
16 plot(log_CA,log_y)
17 xlabel('logCA');ylabel('log(-dCA/dt)')
18 coeff1=regress(log_CA,log_y);
19 n=coeff1(2);
20 k=-10^(coeff1(1));
21 printf("\n After doing linear regression ,the slope
    and intercept of the graph is %f , %f",coeff(2),
    coeff(1))
22 printf("\n The rate equation is therefore given by
    %f",k)
23 printf("CA^1.375 mol/litre.sec")
24 disp('The answer slightly differs from those given
    in book as regress fn is used for calculating
    slope and intercept')

```

Scilab code Exa 3.4 Correct and Incorrect E values

```

1 clear
2 clc
3 // At 400k, -rA=2.3*pA^2
4 //At 500 k, -rA=2.3*pA^2
5 k1=2.3;k2=2.3;T1=400;T2=500;
6 //R=82.06*10^-6 m3.atm/mol.k
7 R=82.06*10^-6;
8 R1=8.314;//m3.pa/mol.k
9 E=(log(k2/k1)*R)/(1/T1-1/T2)

```



```
10 printf("\nRESULT\n")
11 printf("E(J/mol) using pressure units is %f",E)
12 //pA=CA*RT
13 //-rA=2.3(RT)^2*CA^2
14 k1=2.3*(R*T1)^2
15 k2=2.3*(R*T2)^2
16 E=(log(k2/k1)*R1)/(1/T1-1/T2)
17 printf("\nE(J/mol) using concentration units is %f",E
)
```

Chapter 4

Introduction to Reactor Design

Scilab code Exa 4.1 A balance from Stoichiometry

```
1 clear
2 clc
3 // A+3*B gives 6C
4 a=1;b=3;c=6
5 //Initial concentrations
6 CAo=100;CBo=200;Cio=100
7 //Final concentrations
8 CA=40;
9 // Find CB,XA,XB
10 ea=(6-4)/4;
11 XA=(CAo-CA)/(CAo+ea*CA);
12 eb=(ea*CBo)/(b*CAo);
13 XB=b*CAo*XA/CBo;
14 CB=CBo*(1-XB)/(1+eb*XB);
15 printf("\nRESULT\n")
16 printf("The final concentration of B(CB) is %f",CB)
17 printf("\n XA and XB are %f ,%f",XA,XB)
```

Chapter 5

Ideal Reactors for a Single Reaction

Scilab code Exa 5.1 Reaction rate in a mixed flow reactor

```
1 clear
2 clc
3 //Given
4 //Concentrations in mol/litre
5 CAo=0.1; CBo=0.01; Cco=0; CAf=0.02; CBf=0.03; Ccf=0.04;
6 //Volume in litre
7 V=1;
8 //Volumetric flow rate(l/min)
9 v=1;
10 //For mixed flow reactor
11 CA=CAf; CB=CBf; Cc=Ccf;
12 //Rate of reaction(mol/litre.min)
13 rA=(CAo-CA)/(V/v);
14 rB=(CBo-CB)/(V/v);
15 rc=(Cco-Cc)/(V/v);
16 printf("\nRESULT\n")
17 printf("rate of reaction of A(mol/litre.min) is %f\n", rA)
18 printf("\nrate of reaction of B(mol/litre.min) is %f
```

```

    \n",rB)
19 printf("\nrate of reaction of C(mol/litre.min) is %f
    \n",rc)

```

Scilab code Exa 5.2 Kinetics from a mixed flow reactor

```

1 clear
2 clc
3 //Given
4 //Volumetric flow rates(litre/hr)
5 vo=[10;3;1.2;0.5];
6 //Concentrations (millimol/litre)
7 CA=[85.7;66.7;50;33.4];
8 CAo=100;
9 //Volume(litre)
10 V=0.1;
11 //For the stoichiometry 2A—>R
12 //Expansion factor is
13 e=(1-2)/2;
14 //Initialization
15 XA=zeros(4,1);
16 rA=zeros(4,1);
17 //Relation between concentration and conversion
18 for i=1:4
19 XA(i)=(1-CA(i)/CAo)/(1+e*CA(i)/CAo);
20 //Rate of reaction is given by
21 rA(i)=vo(i)*CAo*XA(i)/V;
22 //Testing nth order kinetics
23 //-rA=k*CA^n
24 //log(-rA)=logk+nlog(CA)
25 m(i)=log10(CA(i));
26 n(i)=log10(rA(i));
27 end
28 //For nth order plot between n & m should give a
    straight line

```

```

29 plot(m,n)
30 coefs=regress(m,n);
31 printf("Intercept of the graph is %f\n",coefs(1))
32 printf("Slope of the graph is %f\n",coefs(2))
33 k=10^coefs(1)
34 n=coefs(2)
35 printf("\n Taking n=2,rate of equation(millimol/
    litre.hr) is %f",k)
36 printf("CA^2 \n")
37 disp('The sol slightly differ from that given in
    book because regress fn is used to calculate the
    slope ')

```

Scilab code Exa 5.3 Mixed flow reactor performance

```

1 clear
2 clc
3 //Concentration(mol/litre) of components in the
    mixed feed stream is
4 CAo=1.4;CBo=0.8;CRo=0;
5 //Volume(litre)
6 V=6;
7 //For 75% conversion of B
8 //From stoichiometry of equation A+2B→R
9 CA=1.4-(0.75*0.8)/2;
10 CB=0.8-(0.75*0.8);
11 CR=(0.75*0.8)/2;
12 //From the Given rate equation(mol/litre.min)
13 rB=2*(12.5*CA*CB*CB-1.5*CR);
14 //Volumetric flow rate is given by
15 v=V*rB/(CBo-CB);
16 printf("\n volumetric flow rate(litre/min) into and
    out of the reactor is %f \n",v)
17 disp('The sol varies from book as the value of CB
    taken in book at end is wrong')

```

Scilab code Exa 5.4 Plug flow reactor performance

```
1 clear
2 clc
3 //With 50% inert 2 vol of feed would give 4 vol of
  completely converted gas
4 //Expansion factor is
5 eA=(4-2)/2;
6 //Initial concentration of A(mol/litre)
7 CAo=0.0625;
8 //For 80% conversion
9 xAo=0;xAf=0.8;k=0.01;
10 //For plug flow space time(t) is given by
11 //t=CAo*integral(dxA/-rA)
12 X=integrate('sqrt((1+xA)/(1-xA))','xA',xAo,xAf);
13 t=sqrt(CAo)*X/k;
14 printf("\n Space time(sec) needed is %f \n",t)
```

Scilab code Exa 5.5 Plug flow reactor volume

```
1 clear
2 clc
3 //Given
4 //Temperature(kelvin)
5 T=922;
6 //Pressure(Pascal)
7 P=460000;
8 //Let A=PH3,R=P4,S=H2
9 FAo=40;//mol/hr
10 k=10;//(/hr)
11 R=8.314;
```

```
12 CAo=P/(R*T); // mol/m3
13 e=(7-4)/4;
14 XA=0.8;
15 //The volume of plug flow reactor is given by
16 V=FAo*[(1+e)*log(1/(1-XA))-e*XA]/(k*CAo);
17 printf("\n volume(m3) of reactor is %f \n",V)
```

Scilab code Exa 5.6 Test of a kinetic equation in a plug flow reactor

```
1 clear
2 clc
3 //This is a theoretical Qn
4 printf("Its a theoretical Question")
```

Chapter 6

Design for Single Reactions

Scilab code Exa 6.1 Operating a number of plug flow reactors

```
1 clear
2 clc
3 V1=50;V2=30;V3=40;
4 //Branch D consists of 2 reactor in series ,can be
   considered a single reactor of volume
5 VD=V1+V2;
6 VE=V3;
7 //For Reactor in parallel ,V/F must be same for same
   conversion
8 //VE/FD=VE/VD;FD/F=1/(1+VE/VD)
9 m=VE/VD
10 fr_D=1/(1+m);
11 printf("\n Fraction of feed going to branch D is %f
   \n",fr_D)
```

Scilab code Exa 6.2 Mixed flow reactor in series

```
1 clear
```



```

2  clc
3  //For single reactor and 90% Conversion
4  //From fig 6.6
5  kCot=90;
6  //For 2 reactor space time is doubled and from fig
7  kCot=180;
8  //From graph X=97.4%
9  X=97.4;
10 printf("\\n Part a")
11 printf("\\n The conversion in percentage is %f \\n",X)
12 //For 90% Conversion & N=2.from graph
13 kCot=27.5;
14 //Comparing the reaction rate group for N=1 and N=2,
    We get
15 //(V2/v2)/(V1/v1)=27.5/90
16 //V2=2V1
17 //Ratio of flow rates
18 ratio=90*2/27.5;
19 printf("\\n Part b")
20 printf("\\n Treatment rate can be increased by %f \\n
    ",ratio)

```

Scilab code Exa 6.3 Finding the best reactor set up

```

1  clear
2  clc
3  CAo=[2;5;6;6;11;14;16;24]; //mmol/m3
4  CA=[0.5;3;1;2;6;10;8;4]; //mmol/m3
5  t=[30;1;50;8;4;20;20;4]; //min
6  vo=0.1; //m3/min
7  for i=1:8
8      inv_rA(i)=t(i)/(CAo(i)-CA(i));
9  end
10 //Sorting CA and accordingly changing -1/rA for
    plotting graph between CA and -1/rA

```

```

11 for i=1:8
12     for j=i:8
13         if CA(i)>CA(j)
14             temp=CA(i);
15             CA(i)=CA(j);
16             CA(j)=temp;
17             temp1=inv_rA(i);
18             inv_rA(i)=inv_rA(j);
19             inv_rA(j)=temp1;
20         end
21     end
22 end
23 plot(CA,inv_rA)
24 xlabel('CA(mmol/m3)');ylabel('-1/rA(m3.min/m mol)');
25 disp('From the graph,we can see that we should use
        plug flow with recycle')
26 //From fig
27 CAin=6.6;//mmol/m3
28 R=(10-6.6)/(6.6-1);
29 //V=t*vo=area*vo
30 V=(10-1)*1.2*vo;
31 vr=vo*R;
32 printf("\n Part a")
33 printf("\n The vol of reactor is %f",V)
34 printf("m3 \n The recycle flow rate is %f",vr)
35 printf("m3/min")
36 //Part b,from fig
37 t=(10-1)*10;
38 t1=(10-2.6)*0.8;
39 t2=(2.6-1)*10;
40 //For 1 tank
41 V=t*vo;
42 //For 2 tank
43 V1=t1*vo;
44 V2=t2*vo;
45 Vt=V1+V2;
46 printf("\n Part b")
47 printf("\n For 1 tank volume is %f",V)

```

```
48 printf("m3 \n For 2 tank the volume is %f",Vt)
49 printf("m3")
50 printf("\n Part c")
51 disp('We should use mixed flow followed by plug flow
      ')
52 //For MFR
53 tm=(10-4)*0.2;
54 Vm=tm*vo;
55 //For PFR
56 tp=5.8; //by graphical integration
57 Vp=tp*vo;
58 Vtotal=Vp+Vm;
59 printf("\n For MFR volume(m3) is %f",Vm)
60 printf("\n For PFR volume(m3) is %f",Vp)
61 printf("\n Total volume is %f",Vtotal)
62 printf("m3")
```

Chapter 7

Design for Parallel Reactions

Scilab code Exa 7.1 Contacting patterns for reactions in parallel

```
1 clear
2 clc
3 //Theoretical Questions
4 printf("Its a theoretical Question")
```

Scilab code Exa 7.2 Product distribution for parallel reactions

```
1 clear
2 clc
3 //Initial Concentration(mol/litre) eactant in
  combined feed
4 CAo=10; CBo=10;
5 //For 90% Conversion
6 XA=0.9;
7 CAf=CAo*(1-XA);
8 //Instantaneous fractional yield of desired compound
  is
9 //Q(R/A)=dCR/(dCR+dCS)=CA/(CA+CB^1.5)
```

```

10 //But CA=CB so Q(R/A)=CA/(CA+CA^1.5)
11 //For Plug Flow
12 //Overall Fractional Yield(Qp) is
13 CA=CAf;
14 Qp=(-1/(CAo-CAf))*integrate('1/(1+CA^0.5)', 'CA', CAo,
    CAf);
15 CRf=9*Qp;
16 printf("\n Part a")
17 printf("\n For Plug Flow")
18 printf("\n Concentration of R(mol/litre) in the
    product stream is %f \n", CRf)
19 //Mixed Flow
20 //Overall Fractional Yield(Qm) is
21 Qm=CA/(CA+CA^1.5);
22 CRf=9*Qm;
23 printf("\n Part b")
24 printf("\n For Mixed Flow")
25 printf("\n Concentration of R(mol/litre) in the
    product stream is %f \n", CRf)
26 //Plug flow A, Mixed flow B
27 CAo=19; CB=1;
28 Q=-1/(CAo-CAf)*integrate('CA/(CA+CB^1.5)', 'CA', CAo,
    CAf);
29 CRf=9*Q;
30 printf("\n Part c")
31 printf("\n For Plug flow A, Mixed flow B")
32 printf("\n Concentration of R(mol/litre) in the
    product stream is %f \n", CRf)
33 disp('The result for plug flow varies as there seems
    to be typographical error in integration done in
    book')

```

Scilab code Exa 7.3 Good operating conditions for parallel reactions

```
1 clear
```

```

2  clc
3  CAo=2;
4  //Since S is the desired Product
5  //Q(S/A)=2CA/(1+CA)^2
6  //Part a
7  //Csf=(CAo-CA)*2*CA/(1+CA)^2
8  //on differentiating this to get max Csf,we get max
   value at
9  CA=0.5;
10 Csf=(CAo-CA)*2*CA/(1+CA)^2;
11 printf("\n Part a")
12 printf("\n For Mixed Flow Reactor")
13 printf("\n Maximum expected Cs is %f",Csf)
14 //For Plug Flow Reactor
15 //Production of s is max at 100% Conversion of A
16 CAf=0;
17 Csf=-1*integrate('2*CA/(1+CA)^2','CA',CAo,CAf);
18 printf("\n Part b")
19 printf("\n For Plug Flow")
20 printf("\n Maximum expected concentration of S is %f
   \n",Csf)
21 //Part C
22 //Since no reactant leaves the system unconverted,
   what is important is to operate at condition of
   highest fractional yield
23 //ie. at CA=1 where Q(S/A)=0.5
24 CA=1;
25 Csf=(CAo-CA)*2*CA/(1+CA)^2;
26 printf("Part c")
27 printf("\n For MFR with separation and recycle" )
28 printf("\n Concentration of Csf is %f",Csf)

```

Scilab code Exa 7.4 Best operating conditions for parallel reactions

```
1 clear
```

```
2 clc
3 //Mixed flow followed by plug flow would be best
4 //From ex 7.3
5 //For mixed flow
6 CAo=2; CA=1; Q=0.5;
7 Cs1=Q*(CAo-CA);
8 //For plug flow
9 Cs2=-1*integrate('2*CA/(1+CA)^2','CA',1,0);
10 //Total amount of CS formed is
11 Cs=Cs1+Cs2;
12 printf("Mixed flow followed by plug flow would be
    best")
13 printf("\\n Total amount of CS formed(mol/litre) is
    %f \\n",Cs)
```

Chapter 8

Potpourri of Multiple Reactions

Scilab code Exa 8.1 Favorable contacting patterns for any set of irreversible reactions in series

```
1 clear
2 clc
3 //Theoretical Questions
4 printf("Its a theoretical Question")
```

Scilab code Exa 8.2 Kinetics of series parallel reaction

```
1 clear
2 clc
3 disp('Data is not provided ,only graph is provided')
```

Scilab code Exa 8.3 Evaluate the kinetics from a batch experiment


```

1 clear
2 clc
3 CAo=185;CA=100;t=30;
4 //As A disappears by 1st Order kinetics
5 //ln(CAo/CA)=K123t
6 K123=log(CAo/CA)/t;
7 //From the initial rate of formation of R
8 //dCR/dt(m1)=k2*CAo
9 m1=2;
10 k2=m1/CAo;
11 ////From the initial rate of formation of R
12 m2=1.3;
13 k1=m2/CAo;
14 k3=K123-k1-k2;
15 //Looking at the maxima of S and T curves
16 //For S, Csmax/CAo=(k1/k123)*(k123/k4)^(k4/(k4-k123))
17 //trial and error
18 for k4=0.0001:0.0001:0.1
19     Csmax=CAo*(k1/K123)*((K123/k4)^(k4/(k4-K123)));
20     if Csmax>31.8 & Csmax<32.2
21         break
22     end
23 end
24 //similarly for T
25 for k5=0.001:0.0001:0.02
26     Ctmax=CAo*(k3/K123)*((K123/k5)^(k5/(k5-K123)));
27     if Ctmax>9.95 & Ctmax<10.08
28         break
29     end
30 end
31 printf("\n The rate constants are")
32 printf("\n k1= %f",k1)
33 printf("\n k2= %f",k2)
34 printf("\n k3= %f",k3)
35 printf("\n k4= %f",k4)
36 printf("\n k5= %f",k5)

```

Chapter 9

Temperature and Pressure Effects

Scilab code Exa 9.1 AHr AT VARIOUS TEMPERATURES

```
1 clear
2 clc
3 //Cp values (J/mol.k) given
4 CpA=35; CpB=45; CpR=70;
5 T1=25; T2=1025;
6 Hr=-50000;
7 //Enthalpy balance for 1mol A,1 mol B,2 mol R
8 nA=1; nB=1; nR=2;
9 dH=nA*CpA*(T1-T2)+nB*CpB*(T1-T2)+(Hr)+nR*CpR*(T2-T1)
   ;
10 printf("\n dH(J) at temperature 1025C is %f \n",dH)
11 if dH>0 then
12     printf("Reaction is Exothermic")
13 else
14     printf("Reaction is Endothermic")
15 end
```

Scilab code Exa 9.2 EQUILIBRIUM CONVERSION AT DIFFERENT TEMPERATURES

```
1 clear
2 clc
3 //Standard heat of reaction(J/mol) and Gibbs free
  energy(J/mol)
4 Ho=-75300;Go=-14130;
5 R=8.3214;T1=298;
6 //With all specific heats alike ,dCp=0
7 Hr=-Ho;
8 K298=exp(-Go/(R*T1));
9 //Taking different values of T
10 T1=[2;15;25;35;45;55;65;75;85;95];//degree celcius
11 T=[278;288;298;308;318;328;338;348;358;368];//kelvin
12 for i=1:10
13 K=K298*exp((Hr/R)*((1/T(i))-(1/298)));
14 XAe(i)=K/(K+1);
15 end
16 plot(T1, XAe)
17 xlabel('Temperature(C)')
18 ylabel('XAe')
19 disp(" From the graph we see temp must stay below 78
  C if conversion of 75% or above is expected")
```

Scilab code Exa 9.3 CONSTRUCTION OF THE RATE CONVERSION-TEMPERATURE CHART FROM KINETIC DATA

```
1 clear
2 clc
3 //At 338 k
4 XA=0.581;
5 t=1;//min
6 //From ex 9.2 at 65 degree celcius
7 XAe=0.89;
```

```

8 //For a batch reactor ,k1t/XAe=-ln(1-XA/Xae)
9 k1_338=- (XAe/t)*log(1-(XA/XAe));
10 //At 25 degree celcius
11 XAe1=0.993;
12 T1=338;T2=298;
13 R=8.314;
14 //At 298 k
15 XA1=0.6;
16 t1=10; //min
17 k1_298=- (XAe1/t1)*log(1-(XA1/XAe1));
18 E1=(R*log(k1_338/k1_298))*(T1*T2)/(T1-T2)
19 ko=k1_338/(exp(-E1/(R*T1)))
20 //k1=ko*exp(-E1/RT)
21 //k2=k1/k
22 printf("\n The rate constants are k=exp [(75300/RT)
    -24.7] min-1")
23 printf("\n k1=exp [17.2 -(48900/RT)] min-1")
24 printf("\n k2=exp [41.9 -(123800/RT)] min-1 ")

```

Scilab code Exa 9.4 PERFORMANCE FOR THE OPTIMAL TEMPERATURE PROGRESSION

```

1 clear
2 clc
3 CAo=4; //mol/litre
4 FAo=1000; //mol/min
5 //Drawing locus of max rates on conversion-temp
    graph
6 //tgen drawing optimum path for this system
7 //integrating graphicaaly ,we ger
8 A=0.405; //litre/mol.min
9 t=CAo*A;
10 V=FAo*A;
11 printf("\n Part a")
12 printf("\n The space time needed is %f",t)

```

```

13 printf(" min \n The Volume needed is %f",V)
14 printf(" litres")

```

Scilab code Exa 9.5 OPTIMUM MIXED FLOW REACTOR PERFORMANCE

```

1 clear
2 clc
3 //Concentration of A(mol/litre)
4 CAo=4;
5 //Flow rate of A(mol/min)
6 FAo=1000;
7 XA=0.8;
8 Cp=250; //cal/molA.K
9 Hr=18000; //cal/molA
10 //Using Xa vs T chart of fig 9.3 at 80% conversion
11 //Reaction Rate has the value 0.4 mol/min.litre
12 rA=0.4;
13 //From the performance eqn for mixed flow ,Volume(l)
    is
14 V=FAo*XA/rA;
15 printf("\n Part a")
16 printf("\n The size of reactor(litres) needed is %f"
    ,V)
17 slope=Cp/Hr;
18 //Using graph
19 Qab1=Cp*20; //cal/molA
20 Qab=Qab1*1000; //cal/min
21 Qab=Qab*0.000070; //KW
22 printf("\n Part b")
23 printf("\n Heat Duty(KW) of precooler is %f",Qab)
24 Qce1=Cp*37; //cal/molA fed
25 Qce=Qce1*1000; //cal/min
26 Qce=Qce*0.000070; //KW
27 printf("\n Heat Duty(KW) of postcooler is %f",Qce)

```

Scilab code Exa 9.6 ADIABATIC PLUG FLOW REACTOR PERFORMANCE

```
1 clear
2 clc
3 FAo=1000; //mol/min
4 //Drawing trial operating lines with a slope of 1/72
   and for each evaluating integral dXA/-rA
5 //From graph
6 Area=1.72;
7 V=FAo*Area;
8 printf("\n The volume of adiabatic plug flow reactor
   is %f",V)
9 printf(" litres ")
```

Scilab code Exa 9.7 ADIABATIC PLUG FLOW REACTOR WITH RE-CYCLE I Repeat

```
1 clear
2 clc
3 //Using ex 9.6 and finding optimum recycle area
4 FAo=1000; //mol/min
5 Area=(0.8-0)*1.5;
6 V=FAo*Area;
7 printf("\n The volume required is %f",V)
8 printf(" litre ")
```

Chapter 10

Choosing the Right Kind of Reactor

Scilab code Exa 10.1 THE TRAMBOUZE REACTIONS

```
1 clear
2 clc
3 CAo=1; CA=0.25;
4 v=100 // litre /min
5 ko=.025;k1=0.2;k2=0.4;
6 rA=ko+k1*CA+k2*CA^2;
7 //Volume(litres) per MFR is
8 V=(v/4)*(CAo-CA)/rA;
9 //For 4 Reactor System
10 Vt=4*V;
11 printf("\n The Total volume(lires) of 4 reactor
    system is %f",Vt)
```

Scilab code Exa 10.2 TEMPERATURE PROGRESSION FOR MULTIPLE REACTIONS

```
1 clear
2 clc
3 printf("For Intermediate R is desired")
4 //we want step 1 fast than 2 and step 1 fast than 3
5 printf("\n E1<E2,E1<E3 so use a low temperature and
   plug flow \n")
6 printf("For Product S is desired")
7 //Here speed is all that matters
8 printf("\n High speed is all that matters so use a
   high temperature and plug flow \n")
9 printf("For Intermediate T is desired")
10 //We want step 2 fast than 1 and step 2 fast than 4
11 printf("\n E2>E1,E3>E5 so use a falling temperature
   and plug flow \n")
12 printf("For Intermediate U is desired")
13 //We want step 1 fast than 2 and step 3 fast than 5
14 printf("\n E2>E1,E3>E5 so use a rising temperature
   and plug flow \n")
```

Chapter 11

Basics of Non Ideal Flow

Scilab code Exa 11.1 FINDING THE RTD BY EXPERIMENT

```
1 clear
2 clc
3 //Given Time(min) and Tracer Output Concentration(g/
  litre)
4 T=[0;5;10;15;20;25;30;35];
5 Cpulse=[0;3;5;5;4;2;1;0];
6 dt=5;
7 //Mean Residence time(t)
8 sum1=0;
9 sum2=0;
10 Area=0;//Initialization
11 for i=1:8
12 sum1=sum1+T(i)*Cpulse(i)*dt;
13 sum2=sum2+Cpulse(i)*dt;
14 //Area Under Concentration-Time Curve
15 Area=Area+Cpulse(i)*dt;
16 end
17 t=sum1/sum2;
18 printf("\n The mean residence time(min) is %f \n",t)
19 for j=1:8
20     E(j)=Cpulse(j)/Area;
```

```

21 end
22 plot(T,E)
23 xlabel('time(min)')
24 ylabel('E(min-1)')
25 title('Exit age distribution E vs time')

```

Scilab code Exa 11.2 FINDING THE E CURVE FOR LIQUID FLOW-
ING THROUGH A VESSEL

```

1 clear
2 clc
3 M=150; //Molecular mass(gm)
4 v=5; //litre/sec
5 v=5*60; //litre/min
6 V=860; //litres
7 //From Material Balance
8 Area1=M/v; //gm.min/litre
9 //From the tracer curve
10 A1=0.375;
11 Area2=A1*(1+1/4+1/16+1/64+1/256+1/1024+1/4096); //
    Taking Significant Areas
12 printf("\n From material balance Area(gm.min/litre)
    is %f",Area1)
13 printf("\n From Tracer Curve Area(gm.min/litre) is
    %f",Area2)
14 printf("\n Part a")
15 printf("\n As the two areas are equal,this is a
    properly done experiment \n")
16 //For the liquid ,calculating t
17 sum1=0;
18 for i=1:10
19     sum1=sum1+2*i*A1/(4^(i-1));
20     t=sum1/Area1;
21 end
22 //liquid volume in vessel

```

```

23 V1=t*v;
24 //Fraction of liquid
25 f=V1/V;
26 printf("\n Part b")
27 printf("\n Fraction of liquid is %f",f)
28 //E=Cpulse/M/v
29 printf("\n Part c")
30 printf("\n The E curve is 1.5C")
31 printf("\n Part d")
32 printf("\n The vessel has a strong recirculation of
      liquid ,probably induced by the rising bubbles")

```

Scilab code Exa 11.3 CONVOLUTION

```

1 clear
2 clc
3 //From the given graph
4 Cin(1)=0;Cin(2)=8;Cin(3)=4;Cin(4)=6;Cin(5)=0;
5 E(5)=0;E(6)=0.05;E(7)=0.5;E(8)=0.35;E(9)=0.1;E(10)
   =0;
6 for t=8:14
7 sum1=0;
8 for p=5:t-1
9     if p>10 |(t-p)>5
10         h=2;
11     else
12 sum1=sum1+Cin(t-p)*E(p);
13 Cout(t)=sum1;
14 end
15 end
16 end
17 t=[1:1:14];
18 Cout=Cout';
19 t
20 Cout

```

```
21 plot(t,Cout)
22 xlabel('t');ylabel('Cout')
```

Scilab code Exa 11.4 CONVERSION IN REACTORS HAVING NON IDEAL FLOW

```
1 clear
2 clc
3 k=0.307;
4 //Given mean residence time(min)
5 t=15;
6 //For plug flow with negligible density
7 fr_unconverted=exp(-k*t);
8 printf("\n The fraction of reactant unconverted in a
   plug flow reactor is %f",fr_unconverted)
9 //For the real reactor
10 T=[5;10;15;20;25;30]; //given time
11 E=[0.03;0.05;0.05;0.04;0.02;0.01]; //given
12 dt=5;
13 sum1=0;
14 for i=1:6
15     sum1=sum1+exp(-k*T(i))*E(i)*dt;
16 end
17 printf("\n The fraction of reactant unconverted in a
   real reactor is %f",sum1)
```

Scilab code Exa 11.5 REACTION OF A MACROFLUID

```
1 clear
2 clc
3 k=0.5; //litre/mol.min
4 CAo=2; //mol/litre
5 //From the batch eqn
```

```
6 //CA/CAo=1/(1+kCAo*t)
7 to=1;t1=3;
8 E=0.5;
9 //Using eqn 13
10 XA_avg=1-(E*integrate('1/(1+t)', 't', to, t1));
11 printf("\n Average concentration of A remaining in
    the droplet is %f", XA_avg)
```

Chapter 12

Compartment Models

Scilab code Exa 12.1 BEHAVIOR OF A G L CONTACTOR

```
1 clear
2 clc
3 //First calculating tg and tl from the tracer curves
  (fig E12.1)
4 tg=(8*(9-6)*(0.5)+11*(15-9)*(0.5))/((15-6)*0.5); //
  sec
5 tl=40; //sec
6 vg=0.5; vl=0.1;
7 Vg=tg*vg;
8 Vl=tl*vl;
9 //In terms of void fraction
10 %G=Vg*10; %L=Vl*10; %Stagnant=(100-%G-%L);
11 printf("\n fraction of gas is %f",%G)
12 printf("\n fraction of liquid is %f",%L)
13 printf("\n fraction of Stagnant liquid is %f",
  %Stagnant)
```

Scilab code Exa 12.2 MISBEHAVING REACTOR

```
1 clear
2 clc
3 CAo=1;
4 XA=0.75; //present
5 CA=1-XA;
6 //For mixed flow reactor
7 kt1=(CAo-CA)/CA;
8 //After new setup
9 kt2=3*kt1; //volume is reduced by 1/3
10 CA_unconverted=1/(kt2+1);
11 XA=1-CA_unconverted; //New XA after replacing the
    stirrer
12 printf("\n New Conversion Expected is %f",XA)
```

Chapter 13

The Dispersion Model

Scilab code Exa 13.1 DluL FROM A C CURVE

```
1 clear
2 clc
3 //Time in min
4 T=[0;5;10;15;20;25;30;35];
5 //Tracer Concentration in gm/litre
6 Cpulse=[0;3;5;5;4;2;1;0];
7 //Initialization
8 sum1=0;
9 sum2=0;sum3=0;
10 for i=1:8
11     sum1=sum1+Cpulse(i);
12     sum2=sum2+Cpulse(i)*T(i);
13     sum3=sum3+Cpulse(i)*T(i)*T(i);
14 end
15 ///Mean(min) of continuous distribution
16 t=sum2/sum1;
17 //Variance(min^2) of continuous distribution
18 sigma_sqr=(sum3/sum1)-((sum2/sum1))^2;
19 sigmatheta_sqr=sigma_sqr/t^2;
20 //Calculating vessel dispersion number
21 //Using eqn 13.let  $d/uL=m$ 
```



```

22 for m=0.1:0.001:0.2
23     sigmat_sqr=2*m-2*(m^2)*(1-exp(-(1/m)));
24     if sigmat_sqr >= sigmatheta_sqr
25         break;
26     end
27 end
28 printf("\n The vessel dispersion number is %f",m)

```

Scilab code Exa 13.2 DuL FROM AN F CURVE

```

1 clear
2 clc
3 //length of column(mm)
4 l=1219;
5 //Velocity(mm/s)
6 u=0.0067;
7 //Using the probability graph
8 //16th percentile point fall at
9 t1=178550;
10 //84th percentile point fall at
11 t2=187750;
12 //standard deviation
13 sigma=(t2-t1)/2;
14 t=l/u;
15 sigma_theta=sigma/t;
16 //Vessel dispersion number
17 d=sigma_theta^2/2;
18 printf("\n The vessel dispersion number is %f",d)

```

Scilab code Exa 13.3 DuL FROM A ONE SHOT INPUT

```

1 clear
2 clc

```

```
3 //Bed voidage
4 v=0.4;
5 //Superficial velocity of fluid(cm/s)
6 u=1.2;
7 l=90;//length(cm)
8 //Variance(sec^2) of output signals
9 sigma1_sqr=39;sigma2_sqr=64;
10 dsigma_sqr=sigma2_sqr-sigma1_sqr;
11 //In dimensionless form
12 t=l*v/u;
13 sigmatheta_sqr=dsigma_sqr/t^2;
14 //Dispersion number
15 d=sigmatheta_sqr/2;
16 printf("\n The vessel dispersion number is %f",d)
```

Scilab code Exa 13.4 CONVERSION FROM THE DISPERSION MODEL

```
1 clear
2 clc
3 disp("All the values have to be read from the given
graph")
```

Chapter 14

The Tanks In Series Model

Scilab code Exa 14.1 MODIFICATIONS TO A WINERY

```
1 clear
2 clc
3 //Original and new length(m)
4 L1=32;L2=50;
5 sigma1=8;
6 // For small deviation from plug flow ,sigma_sqr is
   directly proportional to L
7 sigma2=sigma1*sqrt(L2/L1);
8 printf("\n No of bottles of rose expected is %f",
   sigma2)
```

Scilab code Exa 14.2 A FABLE ON RIVER POLLUTION

```
1 clear
2 clc
3 sigma1=14;sigma2=10.5;
4 L1=119;
5 //spread of curve is directly proportional to sqrt
   of distance from origin
```

```

6 L=sigma1^2*L1/(sigma1^2-sigma2^2);
7 printf("\n The dumping of toxic phenol must have
   occurred within %f",L)
8 printf("miles upstream of cincinnati")

```

Scilab code Exa 14.3 F LOW MODELS FROM RTD CURVES

```

1 clear
2 clc
3 vo=1;
4 t1=1/6;
5 t2=1;
6 t3=11/6;
7 w=1/10;
8 //Ratio of areas of the first 2 peaks
9 A2_by_A1=0.5;
10 R=A2_by_A1/(1-A2_by_A1);
11 //From the location of 1st peak
12 V1=(R+1)*vo*t1;
13 //From the time between peaks
14 V2=(R*vo)*((t2-t1)-(t1));
15 //From fig 14.3
16 N=1+(2*(t1/w))^2;
17 printf("\n The reflux ratio is %f",R)
18 printf("\n The volume of 1st tank is %f", V1)
19 printf("\n The volume of 2nd tank is %f",V2)
20 printf("\n The number of tanks are %f ",N)

```

Scilab code Exa 14.4 FINDING THE VESSEL E CURVE USING A SLOPPY TRACER INPUT

```

1 clear
2 clc

```

```

3 //from fig E14.4a
4 t2=280;t1=220;
5 sigma1_sqr=100;sigma2_sqr=1000;
6 dt=t2-t1;
7 dsigma_sqr=sigma2_sqr-sigma1_sqr;
8 N=dt^2/dsigma_sqr;
9 for t=1:200
10 //For N tank in series
11 E(t)=((t^(N-1))*(N^N)*exp(-t*N/dt))/((factorial(N-1)
    )*(dt^N));
12 end
13 for i=1:200
14     t(i)=i;
15 end
16 plot(t,E)
17 xlabel('time(sec)')
18 ylabel('E(sec^-1)')
19 title('Shape of E curve')

```

Chapter 16

Earliness of Mixing Segregation and RTD

Scilab code Exa 16.1 EFFECT OF SEGREGATION AND EARLINESS OF MIXING ON CONVERSION

```
1 clear
2 clc
3 Co=1;k=1;t=1; //given
4 //Scheme A
5 //For mixed flow reactor
6 //t=(Co-C1)/KC1^2
7 C1=(-1+sqrt(1-4*t*(-Co)))/2*t;
8 //For the plug flow reactor
9 //t=1/k(1/C2-1/C1)
10 C2=C1/(1+k*t*C1);
11 printf("\n Conversion for flow scheme A is %f",C2)
12 //Scheme B
13 //For plug flow
14 C3=Co/(1+k*t*Co);
15 //For mixed flow reactor
16 C4=(-1+sqrt(1-4*t*(-C3)))/2*t;
17 printf("\n Conversion for flow scheme B is %f",C4)
18 //Scheme C,D,E
```

```
19 //Using exit age distribution fn for 2 equal plug-  
    mixed flow reactor system, using fig 12.1  
20 t_bar=2;  
21 in=1000;  
22 C5=integrate( '(2/t_bar)*(exp(1-2*t/t_bar))/(1+Co*k*t  
    )', 't', t_bar/2, in);  
23 printf("\n Conversion for flow scheme C,D,E is %f",  
    C5)
```

Chapter 17

Heterogeneous Reactions

Scilab code Exa 17.1 THE BURNING OF A CARBON PARTICLE IN AIR

```
1 clear
2 clc
3 printf("\n Its a theorotical question")
```

Scilab code Exa 17.2 AEROBIC FERMENTATION

```
1 clear
2 clc
3 printf("\n Its a theorotical question")
```

Scilab code Exa 17.3 OVERALL RATE FOR A LINEAR PROCESS

```
1 clear
2 clc
3 printf("\n Its a theorotical question")
```

Scilab code Exa 17.4 OVERALL RATE FOR A NONLINEAR PROCESS

```
1 clear
2 clc
3 printf("\n Its a theorotical question")
```

Chapter 18

Solid Catalyzed Reactions

Scilab code Exa 18.1 SEARCH OF THE RATE CONTROLLING MECHANISM

```
1 clear
2 clc
3 dp=2.4*(10^-3);L=dp/6;
4 //Effective mass conductivity(m3/hr.mcat)
5 De=5*10^-5;
6 //Effective thermal conductivity(KJ/hr.mcat.K)
7 Keff=1.6;
8 //For the gas film surrounding the pellet
9 h=160;//heat transfer coefficient(KJ/hr.m2cat.K)
10 kg=300;//mass transfer coefficient(m3/hr.m2cat)
11 //For the reaction
12 Hr=-160;//KJ/molA
13 CAg=20;//mol/m3
14 rA_obs=10^5;//mol/hr.m3cat
15 kobs=rA_obs/CAg;
16 Vp=3.14*(dp^3)/6;
17 S=3.14*(dp^2);
18 //Observed rate/rate if film resistance controls
19 ratio=kobs*Vp/(kg*S);
20 printf("\n Part a")
```

```

21 if ratio<0.01
22     printf("\n Resistance to mass transport to film
           should not influence rate of reaction")
23 else
24     printf("\n Resistance to mass transport to
           film should influence rate of reaction")
25 end
26 printf("\n Part b")
27
28 Mw=rA_obs*(L^2)/(De*CAg);
29 printf("\n Mw= %f",Mw)
30 if Mw>4
31     printf("\n Pore diffusion is influencing and hence
           strong pore diffusion")
32 else
33     printf("\n Pore diffusion is not influencing
           and hence weak pore diffuusion")
34 end
35 //Temp variation within pellet
36 dt_max_pellet=De*(CAg-0)*(-Hr)/Keff;
37 //Temp variation Across the gas film
38 dt_max_film=L*rA_obs*(-Hr)/h;
39 printf("\n Part c")
40 printf("\n dTmax, pellet is %f",dt_max_pellet)
41 printf(" degree C \n dTmax, film is %f",dt_max_film)
42 printf(" degree C")
43 if dt_max_pellet<1
44     printf("\n Pellet is close to uniform in
           temperature")
45 else
46     printf("\n There is a variation in temp within
           pellet")
47     end
48     if dt_max_film<1
49     printf("\n Film is close to uniform in
           temperature")
50 else
51     printf("\n There is a variation in temp within

```

```

                    Film")
52
53 end

```

Scilab code Exa 18.2 THE RATE EQUATION FROM A DIFFERENTIAL REACTOR

```

1 clear
2 clc
3 // Pressure (atm)
4 PAo=3.2;
5 R=0.082; // litre.atm/mol.k
6 T=390; //k
7 v=20; // litre/hr
8 W=0.01; //kg
9 CA_in=[0.1;0.08;0.06;0.04];
10 CA_out=[0.084;0.07;0.055;0.038];
11 CAo=PAo/(R*T);
12 FAo=CAo*v;
13 eA=3;
14 for i=1:4
15 XA_in(i)=(1-CA_in(i)/CAo)/(1+eA*CA_in(i)/CAo);
16 XA_out(i)=(1-CA_out(i)/CAo)/(1+eA*CA_out(i)/CAo);
17 dXA(i)=XA_out(i)-XA_in(i);
18 rA(i)=dXA(i)/(W/FAo);
19 CA_avg(i)=(CA_in(i)+CA_out(i))/2;
20 end
21 plot(CA_avg,rA)
22 xlabel('CA(mol/litre)')
23 ylabel('-rA(mol/hr.kg)')
24 coeff1=regress(CA_avg,rA)
25 k=coeff1(2)
26 printf("\n The rate of reaction(mol/hr.kg) is %f",k)
27 printf("CA")
28 disp('The answer slightly differs from those given

```

in book as regress fn is used for calculating slope and intercept')

Scilab code Exa 18.3 THE RATE EQUATION FROM AN INTEGRAL REACTOR

```
1 clear
2 clc
3 CAo=0.1; //mol/litre
4 FAo=2; //mol/hr
5 eA=3;
6 CA=[0.074;0.06;0.044;0.029]; //mol/litre
7 W=[0.02;0.04;0.08;0.16]; //kg
8 //Gussing 1st order ,plug flow rxn
9 //(1+eA)*log(1/(1-XA))-eA*XA=k*(CAo*W/FAo)
10 for i=1:4
11 XA(i)=(CAo-CA(i))/(CAo+eA*CA(i));
12 y(i)=(1+eA)*log(1/(1-XA(i)))-eA*XA(i);
13 x(i)=CAo*W(i)/FAo;
14 W_by_FAo(i)=W(i)/FAo;
15 CAout_by_CAo(i)=CA(i)/CAo;
16 XA1(i)=(1-CAout_by_CAo(i))/(1+eA*CAout_by_CAo(i));
17 end
18 plot(x,y)
19 coeff3=regress(x,y);
20 xlabel('CAoW/FAo'),ylabel('4ln(1/1-XA)-3XA')
21 k=coeff3(2);
22 printf("\n Part a, using integral method of analysis"
23 )
24 printf("\n The rate of reaction(mol/litre) is %f",k)
25 printf("CA")
26 //Part b
27 //plotting W_by_FAo vs XA1,the calculating rA=dXA/d(
28 W/FAo) for last 3 points ,we get
29 rA=[5.62;4.13;2.715];
```

```

28 coeff2=regress(CA(2:4),rA);
29 printf("\n Part b,using differential method of
    analysis")
30 printf("\n The rate of reaction(mol/litre) is %f",
    coeff2(2))
31 printf("CA")

```

Scilab code Exa 18.4 PLUG FLOW REACTOR SIZE FROM A RATE EQUATION

```

1 clear
2 clc
3 XA=0.35;
4 FAo=2000; //mol/hr
5 eA=3;k=96;
6 CAo=0.1;
7 W=((1+eA)*log(1/(1-XA))-eA*XA)*(FAo/(k*CAo));
8 printf("\n The amount of catalyst(kg) needed in a
    packed bed reactor is %f",W)

```

Scilab code Exa 18.5 PLUG FLOW REACTOR SIZE FROM RATE CONCENTRATION DATA

```

1 clear
2 clc
3 CAo=0.1;
4 eA=3;
5 rA=[3.4;5.4;7.6;9.1];
6 CA=[0.039;0.0575;0.075;0.092];
7 XA=zeros(4,1);
8 inv_rA=zeros(4,1);
9 for i=1:4
10 XA(i)=(1-CA(i)/CAo)/(1+eA*CA(i)/CAo);

```

```

11 inv_rA(i)=1/rA(i);
12 end
13 //W=FAo*integral(dXA/-rA) from 0 to 0.35
14 //Using Trapezoidal rule to find area ,XA must be in
    increasing order
15 //Sorting XA and accordingly inv_rA
16 for i=1:4
17     small=XA(i);
18     for j=i:4
19         next=XA(j);
20         if small>next
21             temp=XA(i);
22             XA(i)=XA(j);
23             XA(j)=temp;
24             temp1=inv_rA(i);
25             inv_rA(i)=inv_rA(j);
26             inv_rA(j)=temp1;
27         end
28     end
29 end
30 plot(XA,inv_rA)
31 xlabel('XA');ylabel('-1/rA');
32 //extending points to include XA=0.35
33 XA(5)=0.35;inv_rA(5)=0.34;
34 Area=inttrap(XA,inv_rA);
35 W=Area*2000;
36 printf("Amount of catalyst needed(kg) is %f",W)
37 disp('The answer slightly differs from those given
    in book as trapezoidal rule is used for
    calculating area')

```

Scilab code Exa 18.6 MIXED FLOW REACTOR SIZE

```

1 clear
2 clc

```

```
3 XA=0.35;
4 FAo=2000; //mol/hr
5 CAo=0.1 //mol/litre
6 eA=3;k=96;
7 CA=CAo*((1-XA)/(1+eA*XA))
8 rA=k*CA;
9 //For mixed flow
10 W=FAo*XA/rA;
11 printf("The amount of catalyst needed(kg) is %f",W)
```

Scilab code Exa 18.7 MASS TRANSFER RESISTANCES

```
1 clear
2 clc
3 printf("Its a theoretical qn")
```

Chapter 19

The Packed Bed Catalytic Reactor

Scilab code Exa 19.1 DESIGN OF A SINGLE ADIABATIC PACKED BED SYSTEM

```
1 clear
2 clc
3 Cp=40; //J/mol.k
4 Hr=80000; //J/mol.k
5 FAo=100; //mol/s
6 nA=1; nB=7;
7 n=nA+nB;
8 T1=300; //k
9 T2=600; //k
10 T3=800; //k
11 //Slope of adiabatic is
12 m=Cp/Hr;
13 //Drawing various adiabatics on graph given in Fig
    19.11, we get
14 XA=[0.8;0.78;0.7;0.66;0.5;0.26;0.1;0];
15 inv_rA=[20;10;5;4.4;5;10;20;33];
16 plot(XA, inv_rA)
17 xlabel('XA'); ylabel('inv_rA');
```

```

18 disp('From the plot we can say that a recycle
      reactor should be used')
19 W=FAo*XA(1)*6;
20 //From Plot
21 R=1;
22 Q1=n*FAo*Cp*(T2-T1);
23 Q2=n*FAo*Cp*(T1-T3);
24 printf("\n The weight of catalyst needed is %f",W)
25 printf(" kg \n The Recycle Ratio is %f",R)
26 printf("\n The heat exchange for feed is %f",Q1
      /10^6)
27 printf(" MW \n The heat excahge for the product is
      %f",Q2/10^6)
28 printf(" MW")

```

Scilab code Exa 19.2 DESIGN OF A TWO ADIABATIC PACKED BED SYSTEM

```

1 clear
2 clc
3 Cp=40;
4 Hr=80000;
5 m=Cp/Hr;
6 FAo=100;//mol/s
7 //Drawing various adiabatics on graph given in Fig
      19.11,
8 //We see from fig E 19.2 a ,that this gives very
      shallow adiabatic,As rate continually increase as
      you move along htis adiabatic
9 disp('We should use a mixed flow reactor operating
      at optimum ')
10 XA=[0.85;0.785;0.715;0.66;0.58;0.46];
11 inv_rAopt=[20;10;5;3.6;2;1];
12 plot(XA,inv_rAopt)
13 xlabel('XA');ylabel('rA^-1');

```

```

14 //Using method of maximization of rectangles
15 area1=0.66*3.6;
16 area2=(0.85-0.66)*20;
17 W1=FAo*area1;
18 W2=FAo*area2;
19 printf("\n The weight of catalyst needed for 1st bed
      is %f",W1)
20 printf("kg \n The weight of catalyst needed for 2
      ndbed is %f",W2)
21 printf("kg")
22 //Heat exchange
23 //For the first reactor
24 //To go to 66% conversion at 820 degree C,the amount
      of heat needed per mol of A is
25 Q=(820-300)*Cp+0.66*(-Hr);
26 //For 100 mol/s
27 Q1= FAo*Q/10^6; //MW
28 printf("\n The amount of heat exchanged for 1st
      reactor is %f",Q1)
29 printf("MW")
30 //For 2nd reactor
31 //To go from XA=0.66 at 820 k to XA=0.85 at 750 k
32 Q2=FAo*((750-820)*Cp+(0.85-0.66)*(-Hr));
33 Q2=Q2/10^6;
34 printf("\n The amount of heat exchanged for 2nd
      reactor is %f",Q2)
35 printf("MW")
36 //For the exchanger needed to cool the exit stream
      from 750 k to 300 k
37 Q3=FAo*Cp*(300-750);
38 Q3=Q3/10^6; //MW
39 printf("\n The amount of heat exchanged for
      exchanger is %f",Q3)
40 printf("MW")

```

Chapter 20

Reactors with Suspended Solid Catalyst Fluidized Reactors of Various Types

Scilab code Exa 20.1 First Order Catalytic Reaction in a BFB

```
1 clear
2 clc
3 uo=0.3;umf=0.03;//m/s
4 vo=0.3*3.14159;//m3/s
5 d=2;//m
6 db=0.32;//dia of bubble(m)
7 emf=0.5;
8 W=7000;//kg
9 CAo=100;//mol/m3
10 D=20*10^-6;//m2/s
11 density=2000;//kg/m3
12 k=0.8;
13 alpha=0.33;
14 g=9.8;//m/s2
15 //Using bubbling bed model
16 //Rise velocity of bubbles
17 ubr=0.711*sqrt(g*db);
```

```

18 ub=uo-umf+ubr;
19 delta=uo/ub;
20 ef=1-(1-emf)*(1-delta);
21 Kbc=4.5*(umf/db)+5.85*(D^0.5)*(g^0.25)/(db^1.25);
22 Kce=6.77*sqrt(emf*D*ubr/db^3);
23 fb=0.001;
24 fc=delta*(1-emf)*((3*umf/emf)/(ubr-umf/emf)+alpha);
25 fe=(1-emf)*(1-delta)-fc-fb;
26 ft=fb+fe+fc;
27 A=3.14*d*d/4;
28 Hbfb=W/((density*A)*(1-ef));
29 XA=1-inv(exp(fb*k+(1/((1/(delta*Kbc))+1/((fc*k)
      +(1/((1/(delta*Kce))+1/(fe*k)))))))*(Hbfb*ft/uo)
      /ft));
30 XA1=100*XA; //in percentage
31 printf("\n Part a")
32 printf("\n Conversion of reactant is %f ",XA1)
33 CA_avg=CAo*XA*vo*density/(k*W);
34 printf("\n Part b")
35 printf("\n The proper mean concentration (mol/m3) of
      A seen by solid is %f",CA_avg)
36 XA1=1-inv(exp(k*ft*Hbfb/uo));
37 printf("\n Part c")
38 printf("\n Conversion of reactant for packed bad is
      %f",XA1)

```

Chapter 21

Deactivating Catalysts

Scilab code Exa 21.1 INTERPRETING KINETIC DATA IN THE PRESENCE OF PORE DIFFUSION RESISTANCE AND DEACTIVATION

```
1 clear
2 clc
3 t=[0;2;4;6];
4 XA=[0.75;0.64;0.52;0.39];
5 t1=4000; //kg.s/m3
6 density_s=1500; //kg/m3
7 De=5*10^-10;
8 d=2.4*10^-3;
9 // Assuming -rA=kCA*a, -da/dt=kd*a
10 // For this rate a plot of ln(CAo/CA-1) vs t should
   give a straight line
11 for i=1:4
12     y(i)=log((1/(1-XA(i)))-1);
13 end
14 plot(y,t)
15 xlabel('t')
16 ylabel('ln(CAo/CA-1)')
17 // Guessing No Intrusion of Diffusional Resistance
18 // ln(CAo/CA-1)=ln(k*t1)-kd*t
19 coeff =regress(t,y);
```

```

20 kd=coeff(2);
21 k=exp(coeff(1))/t1;
22 L=d/6;
23 Mt=L*sqrt(k*density_s/De);
24 //Assuming Runs were made in regime of strong
    resistance to pore diffusion
25 k1=((exp(coeff(1)))^2)*(L^2)*density_s/(t1*t1*De);
26 kd1=-2*coeff(2);
27 Mt=L*sqrt(k1*density_s/De);
28 printf("\n Rate equation(mol/kg.s) in diffusion free
    regime with deactivation is %f ",k1)
29 printf("CA*a with \n -da/dt(hr-1) is %f",kd1)
30 printf("a")
31 //In strong pore diffusion
32 k2=k1*sqrt(De/(k1*density_s));
33 printf("\n Rate equation(mol/kg.s) in strong pore
    diffusion resistance regime with deactivation is
    %f ",k2)
34 printf("CA*a^0.5/L with \n -da/dt(hr-1) is %f",kd1)
35 printf("a")

```

Scilab code Exa 21.2 DEACTIVATION IN A PACKED BED REACTOR

```

1 clear
2 clc
3 PAo=3; //atm
4 R=82.06*10^-6; //m3.atm/mol.k
5 T=730; //k
6 W=1000; //kg
7 FAo=5000; //mol/hr
8 CAo=PAo/(R*T);
9 tau=W*CAo/FAo;
10 i=0;
11 for t=0:5:120
12     i=i+1;

```

```

13 //Part a
14 a(i)=1-(8.3125*10^-3)*t;
15 XA(i)=(tau^2)*a(i)/(1+(tau^2)*a(i));
16 //Part b
17 a1(i)=exp(-0.05*t);
18 XA1(i)=(tau^2)*a1(i)/(1+(tau^2)*a1(i));
19 //Part c
20 a2(i)=1/(1+3.325*t);
21 XA2(i)=(tau^2)*a2(i)/(1+(tau^2)*a2(i));
22 //Part d
23 a3(i)=1/(sqrt(1+1333*t));
24 XA3(i)=(tau^2)*a3(i)/(1+(tau^2)*a3(i));
25 end
26 t=[0:5:120];
27 plot(t,XA,t,XA1,t,XA2,t,XA3)
28 xlabel('Time(days)')
29 ylabel('XA')
30 legend('Zero Order','1st Order','2nd Order','3rd
        Order');
31 XA_avg=(1/120)*integrate('(100*(1-(8.3125*10^-3)*t))
        /(1+100*(1-(8.3125*10^-3)*t))','t',0,120);
32 XA1_avg=(1/120)*integrate('(100*exp(-0.05*t))
        /(1+100*exp(-0.05*t))','t',0,120);
33 XA2_avg=(1/120)*integrate('(100*(1/(1+3.325*t)))
        /(1+100*(1/(1+3.325*t)))','t',0,120);
34 XA3_avg=(1/120)*integrate('(100*1/(sqrt(1+1333*t)))
        /(1+100*(1/sqrt(1+1333*t)))','t',0,120);
35 printf("\n for d=0,the mean conversion is % f",
        XA_avg)
36 printf("\n for d=1,the mean conversion is % f",
        XA1_avg)
37 printf("\n for d=2,the mean conversion is % f",
        XA2_avg)
38 printf("\n for d=3,the mean conversion is % f",
        XA3_avg)

```

Chapter 22

GL Reactions on Solid Catalysts

Scilab code Exa 22.1 HYDROGENATION OF ACETONE IN A PACKED BUBBLE COLUMN

```
1 clear
2 clc
3 PA=101325; //Pa
4 HA=36845; //PA.m3.l/mol
5 CBo=1000; //mol/m3
6 v=10^-4; //m3*l/s
7 h=5; //m
8 A=0.1; //m2
9 CA=PA/HA;
10 FBo=v*CBo;
11 Vr=A*h;
12 dp=5*10^-3; //mcat
13 d_solid=4500; //kg/m3cat
14 De=8*10^-10; //m3l/mcat.s
15 n=0.5;
16 b=1;
17 k=2.35*10^-3;
18 L=dp/6;
```

```

19 kai_overall=0.02;
20 kac_ac=0.05;
21 f=0.6;
22 //For a half-order reaction
23 Mt=L*sqrt((n+1)*(k*d_solid*(CA)^(n-1))/(2*De));
24 E=1/Mt;
25 rA=(1/((1/(kai_overall))+1/(kac_ac))+1/(k*b*(CA^(n
    -1))*E*f*d_solid))))*(PA/HA);
26 //From Material Balance
27 XB=b*rA*Vr/FBo;
28 printf("\n The conversion of acetone is %f",XB)

```

Scilab code Exa 22.2 HYDROGENATION OF A BATCH OF BUTYNE-DIOL IN A SLURRY REACTOR

```

1 clear
2 clc
3 PA=14.6*101325; //Pa
4 HA=148000;
5 Vr=2;
6 Vl=Vr;
7 b=1;
8 fs=0.0055;
9 k=5*10^-5; //m6l/kg.molcat.s
10 dp=5*10^-5; //mcat
11 kac=4.4*10^-4; kai=0.277; //m3l/m3.r.s
12 density=1450; //kg/m3
13 De=5*10^-10; //m3l/mcat.s
14 L=dp/6; //for spherical particle
15 CA=PA/HA;
16 X=0.9;
17 CBo=2500; //mol/m3.l
18 CB=CBo*(1-X);
19 ac=6*fs/dp;;
20 K=kac*ac;

```

```

21 //Guessing different values of CB
22 CB=[2500;1000;250];
23 e=[0.19;0.29;0.5];
24 for i=1:3
25     Mt(i)=L*sqrt(k*CB(i)*density/De);
26     rA(i)=CA/((1/kai)+(1/K)+(1/(k*density*e(i)*fs*CB
        (i))))
27     inv_rA(i)=1/rA(i);
28 end
29 plot(CB,inv_rA)
30 xlabel('CB');ylabel('-1/rA')
31 //Reaction time is given by (Vl/b*Vr)*integral(dCB/-
    rA)
32 //Graphically integrating
33 Area=3460;
34 t=Vl*Area/(b*Vr);
35 t=t/60;//min
36 printf("\n The time required for 90 percentage
    conversion of reactant is %f",t)
37 printf("min")

```

Chapter 23

Fluid Fluid Reactions Kinetics

Scilab code Exa 23.1 FINDING THE RATE OF A GL REACTION

```
1 clear
2 clc
3 k=10^6;
4 Kag_a=0.01; f1=0.98;
5 Kal=1;
6 HA=10^5;
7 DA1=10^-6;
8 DB1=DA1;
9 PA=5*10^3; //Pa
10 CB=100; //mol/m3
11 b=2;
12 a=20; //m2/m3
13 Mh=sqrt(DA1*k*CB*CB)/Kal;
14 Ei=1+(DB1*CB*HA/(b*DA1*PA));
15 E=100;
16 printf("\n Part a")
17 res_total=((1/(Kag_a))+(HA/(Kal*a*E))+(HA/(k*CB*CB*
    f1))));//Total Resistance
18 f_gas=(1/(Kag_a))/res_total;//fraction of resistance
    in gas film
19 f_liq=(HA/(Kal*a*E))/res_total;//fraction of
```

```

    resistance in liquid film
20 printf("\n Fraction of the resistance in the gas
    film is %f",f_gas)
21 printf("\n Fraction of the resistance in the liquid
    film is %f",f_liq)
22 printf("\n Part b")
23 printf("\n The reaction zone is in the liquid film")
24 printf("\n Part c")
25 if Ei>5*Mh
26     printf("\n We have pseudo 1st order reaction in
        the film")
27 end
28 //From fig 23.4
29
30 rA=PA/(((1/(Kag_a))+(HA/(Kal*a*E))+(HA/(k*CB*CB*f1))
    ));
31 printf("\n Part d")
32 printf("\n The rate of reaction (mol/m3.hr) is %f",rA
    )

```

Chapter 24

Fluid Fluid Reactors Design

Scilab code Exa 24.1 TOWERS FOR STRAIGHT ABSORPTION

```
1 clear
2 clc
3 kag_a=0.32; // mol/hr.m3.Pa
4 kal_a=0.1; // hr
5 HA=12.5; // Pa.m3/mol
6 Fg=10^5; // mol/hr.m2
7 Fl=7*10^5; // mol/hr.m2
8 Ct=56000; // mol/m3
9 P=10^5; // Pa
10 //pA3-pA1=(Fl*P)*(CA3-CA1)/(Fg*CT)
11 //CA3=0.08*PA3-1.6
12 inv_Kag_a=inv(kag_a)+HA/(kal_a);
13 Gfilm_res=(inv(kag_a))/inv_Kag_a;
14 Lfilm_res=(HA/(kal_a))/inv_Kag_a;
15 Kag_a=1/inv_Kag_a;
16 //d=PA-PA*
17 //p=PA-HA*(0.08*PA-1.6);
18 d=20;
19 h=(Fg/(P*Kag_a))*integrate('1/20','dp',20,100);
20 printf("\n The height of the tower required for
    countercurrent operations is % f",h)
```

```
21 printf("m")
```

Scilab code Exa 24.2 TOWERS FOR HIGH CONCENTRATION OF LIQUID REACTANT

```
1 clear
2 clc
3 Fg=10^5;
4 P=10^5;
5 Fg_by_Acs=10^5; //(Fg/Acs)
6 PA1=20;PA2=100;
7 kag_a=0.32;
8 //rA=kag_a*P
9 //Height of Tower
10 //h=((Fg/Acs)*integral(dPA/rA))/P
11 h=(Fg_by_Acs/P)*integrate('1/(0.32*PA)', 'PA', PA1, PA2
    );
12 printf("\n The height of the tower is %f ",h)
13 printf("m")
```

Scilab code Exa 24.3 TOWERS FOR LOW CONCENTRATION OF LIQUID REACTANT CASE A

```
1 clear
2 clc
3 Fg=10^5;
4 P=10^5;
5 PA1=20;PA2=100;
6 HA=12.5;
7 kaga=0.32;kla=0.1;
8 //CB=(420-PA3)/12.5;
9 //rA=((HA*CB)+pA)/((1/kaga)+(HA/kla))
10 rA=420/((1/kaga)+(HA/kla));
```

```

11 h=(Fg/P)*integrate('1/rA','PA',PA1,PA2);
12 printf("The height of the tower is %f",h)
13 printf("m")

```

Scilab code Exa 24.4 TOWERS FOR INTERMEDIATE CONCENTRATIONS OF LIQUID REACTANT

```

1 clear
2 clc
3 //Using material balance,we have
4 //PA3=1620-12.5*CB3
5 PA1=20;PA2=100;//Pa
6 Fg_by_Acs=10^5;
7 P=10^5;
8 HA=12.5;
9 kaga=0.32;kla=0.1;
10 //Form of rate eqn changes at PA=39.5 Pa
11 PA=39.5;//Pa
12 //h=((Fg/Acs)*integral(dPA/rA))/P
13 h=(Fg_by_Acs/P)*(integrate('1/(kaga*P)','P',PA1,PA)+
    integrate('((1/kaga)+(HA/kla))/1620','PA',PA,PA2)
    );
14 printf("The height of the tower is %f",h)
15 printf("m")

```

Scilab code Exa 24.5 REDO EXAMPLE 24 2 BY THE GENERAL METHOD

```

1 clear
2 clc
3 Fg=10^5;
4 P=10^5;
5 Fg_by_Acs=10^5;//(Fg/Acs)
6 PA1=20;PA2=100;

```



```

7 kag_a=0.32;
8 //Height of Tower
9 //h=((Fg/Acs)*integral(dPA/rA))/P
10 //rA=(1/(3.125+125/E))*PA;
11 //Taking E=infinity ,rA=pA/3.125
12 h=(Fg_by_Acs/P)*integrate('1/(PA/3.125)', 'PA', PA1,
    PA2);
13 printf("\n The height of the tower is %f ",h)
14 printf("m")

```

Scilab code Exa 24.6 REACTION OF A BATCH OF LIQUID

```

1 clear
2 clc
3 kag_a=0.72;
4 kal_a=144;
5 HA=1000;
6 Fg=9000; //mol/hr
7 fl=0.9; b=1;
8 Vr=1.62; //m3
9 DA=3.6*10^-6; //m2/hr
10 a=100; //m2/m3
11 k=2.6*10^5; //m3/mol.hr
12 DB=DA;
13 P=10^5; PA=1000; //Pa
14 kal=kal_a/a;
15 //At the start
16 CBo=555.6;
17 Mh=(sqrt(DB*k*CBo))/kal;
18 //Min value of EAi
19 Ei=1+(CBo*HA/PA);
20 if Ei>Mh
21     E=Mh;
22 end
23 rA1=PA/((P*Vr/Fg)+(1/kag_a)+(HA/(kal_a*E)))+(HA/(k*fl

```

```

    *CBo)));
24 //At the end
25 CBf=55.6;
26 Mh=(sqrt(DB*k*CBf))/ka1;
27 //Min value of EAi
28 Ei=1+(CBf*HA/PA);
29 if Ei>Mh
30     E=Mh;
31 end
32 rA2=PA/((P*Vr/Fg)+(1/kag_a)+(HA/(ka1_a*E))+(HA/(k*f1
    *CBf)));
33 //Average rate of reaction
34 rA_avg=(rA1+rA2)/2;
35 t=(f1/b)*integrate('1/rA_avg','CB',CBf,CBo);
36 printf("\n Part a")
37 printf("\n The run time needed is %f",t)
38 printf(" hr")
39 //The min time required is
40 tmin=Vr*(CBo-CBf)/(Fg*(PA/(P-PA)));
41 printf("\n The minimum time required is %f",tmin)
42 printf(" hr")
43 //Fraction of reactant which passes through the tank
    unreacted is
44 f=(t-tmin)/tmin;
45 printf("\n Part b")
46 printf("\n Fraction of reactant which passes through
    the tank unreacted is %f",f)

```

Chapter 26

Fluid Particle Reactors Design

Scilab code Exa 26.1 CONVERSION OF A SIZE MIXTURE IN PLUG FLOW

```
1 clear
2 clc
3 // Lets say F(Ri)/F=F_ri
4 F_50=0.3;F_100=0.4;F_200=0.3;
5 //The time required(min)for 3 size of particles is
6 t_50=5;t_100=10;t_200=20;
7 //Cosidering solids to be in plug flow with tp=8 min
8 tp=8;
9 //1-XBavg=[1-XB(50 um)]F(50 um)/F+ [1-XB(100 um)]F
    (100 um)/F+.....
10 //Because for 3 sizes of particles ,R1:R2:R3=t1:t2:t3
11 //From eqn 25.23,[1-XB(Ri)]=(1-tp/t(ri))^3
12 a=((1-(tp/t_50))^3)*F_50;b=((1-(tp/t_100))^3)*F_100;
    c=((1-(tp/t_200))^3)*F_200;
13 g=[a,b,c];
14 sum1=0;
15 for p=1:3
16     if g(p)>0
17         sum1=sum1+g(p);
18     end
```

```

19 end
20 f_converted=1-sum1;
21 printf("\n The fraction of solid converted equals %f
      ",f_converted)

```

Scilab code Exa 26.2 CONVERSION OF A SINGLE SIZED FEED IN A MIXED FLOW REACTOR

```

1 clear
2 clc
3 t_avg=60;t=20; //min
4 //For chemical rxn controlling , t =kR
5 unconverted=((1/4)*(t/t_avg))-((1/20)*(t/t_avg)^2)
      +((1/120)*(t/t_avg)^3);
6 //For ash layer diffusion controlling ,t=k1R^2
7 unconverted1=((1/5)*(t/t_avg))-((19/420)*(t/t_avg)
      ^2)+((41/4620)*(t/t_avg)^3);
8 c_avg=(unconverted+unconverted1)/2;
9 printf("Fraction of original sulfide ore remain
      unconverted is %f",c_avg)

```

Scilab code Exa 26.3 CONVERSION OF A FEED MIXTURE IN A MIXED FLOW REACTOR

```

1 clear
2 clc
3 F=1000; //gm/min
4 W=10000; //gm
5 t_avg=W/F;
6 F_50=300;F_100=400;F_200=300; //gm/min
7 t_50=5;t_100=10;t_200=20; //min
8 unconverted=((((1/4)*(t_50/t_avg))-((1/20)*(t_50/
      t_avg)^2)+((1/120)*(t_50/t_avg)^3))*(F_50/F))

```

```

+(((1/4)*(t_100/t_avg))-((1/20)*(t_100/t_avg)^2)
+((1/120)*(t_50/t_avg)^3))*(F_100/F))+(((1/4)*(
t_200/t_avg))-((1/20)*(t_200/t_avg)^2)+((1/120)*(
t_50/t_avg)^3))*(F_200/F));
9 converted=1-unconverted;
10 printf("The mean conversion of soild is %f",
converted)
11 printf("\n The answer slightly differs from those
given in book as we have considered only
significant terms in infinite series")

```

Scilab code Exa 26.4 FINDING THE SIZE OF A FLUIDIZED BED

```

1 clear
2 clc
3 t1=1; //hr
4 //t=k*(1/CAo)
5 //For equal stoichiometric feed XA=XB=0.9
6 //CAf/CAo=0.1
7 t2=t1/0.1;
8 //finding t/t_avg which gives XB=0.9 ie 1-XB=0.1
9 for a=0:0.0001:1;
10     //x=1-XB
11 x=(1/4)*(a)-((1/20)*(a)^2)+((1/120)*(a)^3);
12 if x >0.099 & x<0.1005
13     r=a;
14 end
15 end
16 FBo=1; //tons/hr
17 t_avg=t2/r;
18 W=t_avg*FBo;
19 printf("\n The needed weight of bed is %f",W)
20 printf(" tons")

```

Chapter 29

Substrate Limiting Microbial Fermentation

Scilab code Exa 29.1 MIXED REACTORS FOR MONOD KINETICS

```
1 clear
2 clc
3 printf("\n Its a theorotical qn")
```

Scilab code Exa 29.2 PLUG FLOW REACTOR FOR MONOD KINETICS

```
1 clear
2 clc
3 printf("\n Its a theorotical qn")
```

Scilab code Exa 29.3 GLUCOSE FOR E COLI BACTERIA

```
1 clear
```

```

2  clc
3  CAo=6; CM=0.4; //kg/m3
4  V=1; //m3
5  k=4;
6  //From fig 29.5
7  N=sqrt(1+(CAo/CM));
8  kt_op=N/(N-1);
9  C_by_A=0.1;
10 t_op=kt_op/k;
11 v_op=V/t_op;
12 //The feed rate of glucose
13 FAo=v_op*CAo;
14 printf("\n The feed rate of glucose is %f",FAo)
15 printf("kg/hr")
16 //Max consumption rate of glucose is
17 XA=N/(N+1);
18 c_max=FAo*XA;
19 printf("\n Max consumption rate of glucose is %f ",
        c_max)
20 printf("kg/hr")
21 //Max production rate of E.coli is
22 Cc_op=(C_by_A)*CAo*N/(N+1);
23 Fcmax=v_op*Cc_op;
24 printf("\n Max production rate of E.coli is %f",
        Fcmax)
25 printf("kg/hr")

```

Chapter 30

Product Limiting Microbial Fermentation

Scilab code Exa 30.1 FRUIT FLY COCKTAIL

```
1 clear
2 clc
3 k=sqrt(3); //hr^-1
4 n=1;
5 V=30; //m3
6 CR=0.12; //kgalc/kg sol
7 density=1000; //kg/m3
8 //CR in kg/m3
9 CR=CR*density;
10 CR_opt=CR/2;
11 alcohol_per=CR_opt*100/density; //PErcentage of
    alcohol
12 printf("\n The Percentage of alchol in cocktail is
    %f", alcohol_per)
13 //From fig 30.4
14 kt=1;
15 t=kt/k;
16 t_opt=2*t;
17 v_opt=V/t_opt;
```



```
18 printf("\n The Optimum feed rate is %f",v_opt)
19 printf(" m3/hr")
20 //The production rate of alcohol
21 FR=v_opt*CR_opt;
22 printf("\n The production rate of alcohol is %f ",FR
    )
23 printf(" kgalc/hr")
```
