Scilab Textbook Companion for Chemical Reaction Engineering by O. Levenspiel[1]

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Book Description

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Scilab numbering policy used in this document and the relation to the above book.

Exa Example (Solved example)

Eqn Equation (Particular equation of the above book)

AP Appendix to Example(Scilab Code that is an Appednix to a particular Example of the above book)

For example, Exa 3.51 means solved example 3.51 of this book. Sec 2.3 means a scilab code whose theory is explained in Section 2.3 of the book.

Contents

List of Scilab Codes

Chapter 1

Overview of Chemical Reaction Engineering

Scilab code Exa 1.1 The Rocket Engine

```
clear
clc
//l=75 cm,d=60 cm,H20 Produced=108kg/s
l=0.75;d=0.6;
V=(3.14*d*d*l)/4;
//H2+0.5*O2=H2O
//Molecular wt of H2O=18
M=18;
//H2O Produced in kmol/s
H20_produced=108/M;
//H2 used
H2_used=H20_produced;
//O2 Used
O2_used=0.5*H20_produced;
//Rate of reaction
//Rate of reaction of H2(mol/m^3.s)
r_H2=(H2_used/V)*1000;
//Rate of reaction of O2(mol/m^3.s)
r_O2=(O2_used/V)*1000;
```

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

Scilab code Exa 1.2 The Living Person

```
clear
clc
 // Assuming density of a person=1000kg/m3
 d=1000;
 mass=75;
 V=mass/d;
 //moles of O2 consumed per day
 O2_used=(6000/2816)*6;
 // Rate of reaction (mol/m3.s)
 r_O2=(O2_used/V)/(24*3600);
 printf("\nRESULT\n")
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 reactiom mechanism

```
clear
clc
//Theorotical Questions
printf("Its a theorotical Question")
```

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

```
clear
clc
//Theorotical Questions
printf("Its a theorotical Question")
```

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

```
clear
clc
// Given
//t1=30 min ;T1=336 k;
//t2=15 sec ;T2=347 k;
// Converting t2 in min
t1=30;T1=336;t2=0.25;T2=347
R=8.314;
//log(t1/t2)=E(1/T1-1/T2)/R
E=(log(t1/t2)*R)/(1/T1-1/T2);
printf("\nRESULT\n")
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

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

```
//Guessing nth order kinetics and using fractional life method with F=80%
//log Tf=log(0.8^(1-n)-1/(k(n-1)))+(1-n)logCAo
//plot(t,C_A)

//Picking different values of CAo
//Time needed for 3 runs,,from graph
T=[18.5;23;35];
CAo=[10;5;2];
for i=1:3
    CA(i)=0.8*CAo(i);
    log_Tf(i)=log10(T(i));
    log_CAo(i)=log10(CAo(i));
end
plot(log_CAo,log_Tf)
xlabel('log CAo');ylabel('log t');
coeff1=regress(log_CAo,log_Tf);
n=1-coeff1(2);
printf("From graph we get slope and intercept for calculating rate eqn")
k1=((0.8^(1-n))-1)*(10^(1-n))/(18.5*(n-1));
printf("\n The rate equation is given by %f",k1)
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

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

```
=[-0.1333;-0.1031;-0.0658;-0.0410;-0.0238;-0.0108;-0.0065];
//Guessing nth rate order
//rA=kCA^n
//log(-dCA/dt)=logk+nlogCA
for i=1:7
log_y(i)=log10(y(i));
log_CA(i)=log10(CA(i));
end
plot(log_CA,log_y)
xlabel('logCA');ylabel('log(-dCA/dt)')
coeff1=regress(log_CA,log_y);
n=coeff1(2);
k=-10^(coeff1(1));
printf("\n After doing linear regression,the slope
    and intercept of the graph is %f , %f",coeff(2),
    coeff(1))
printf("\n The rate equation is therefore given by
    %f",k)
printf("CA^1.375 mol/litre.sec")
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

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

```
printf("\nRESULT\n")
printf("E(J/mol)using pressure units is %f",E)
//pA=CA*RT
//-rA=2.3(RT)^2*CA^2
k1=2.3*(R*T1)^2
k2=2.3*(R*T2)^2
E=(log(k2/k1)*R1)/(1/T1-1/T2)
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

```
clear
clc
// A+3*B gives 6C
a=1;b=3;c=6
 //Initial concentrations
 CAo=100;CBo=200;Cio=100
 //Final concentrations
 CA=40;
 // Find CB,XA,XB
 ea=(6-4)/4;
 XA=(CAo-CA)/(CAo+ea*CA);
 eb=(ea*CBo)/(b*CAo);
 XB=b*CAo*XA/CBo;
 CB=CBo*(1-XB)/(1+eb*XB);
 printf("\nRESULT\n")
printf("The final concentration of B(CB) is %f",CB)
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

```
clear
clc
//Given
//Concentrations in mol/litre
CAo=0.1;CBo=0.01;Cco=0;CAf=0.02;CBf=0.03;Ccf=0.04;
//Volume in litre
V=1;
//Volumetric flow rate(l/min)
v=1;
//For mixed flow reactor
CA=CAf;CB=CBf;Cc=Ccf;
//Rate of reaction(mol/litre.min)
rA=(CAo-CA)/(V/v);
rB=(CBo-CB)/(V/v);
rc=(Cco-Cc)/(V/v);
printf("\nRESULT\n")
printf("rate of reaction of A(mol/litre.min) is %f\n
    ",rA)
printf("\nrate of reaction of B(mol/litre.min) is %f
```

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

Scilab code Exa 5.2 Kinetics from a mixed flow reactor

```
clear
clc
//Given
//Volumetric flow rates(litre/hr)
vo=[10;3;1.2;0.5];
//Concentrations (millimol/litre)
CA=[85.7;66.7;50;33.4];
CAo=100;
//Volume(litre)
V=0.1;
//For the stoichiometry 2A—>R
//Expansion factor is
e=(1-2)/2;
//Initialization
XA=zeros(4,1);
rA=zeros(4,1);
//Relation between concentration and conversion
for i=1:4
XA(i)=(1-CA(i)/CAo)/(1+e*CA(i)/CAo);
//Rate of reaction is given by
rA(i)=vo(i)*CAo*XA(i)/V;
//Testing nth order kinetics
//-rA=k*CA^n
//log(-rA)=logk+nlog(CA)
m(i)=log10(CA(i));
n(i)=log10(rA(i));
end
//For nth order plot between n & m should give a
    straight line
```

```
plot(m,n)
coefs=regress(m,n);
printf("Intercept of the graph is %f\n",coefs(1))
printf("Slope of the graph is %f\n",coefs(2))
k=10^coefs(1)
n=coefs(2)
printf("\n Taking n=2,rate of equation(millimol/
   litre.hr) is %f",k)
printf("CA^2 \n")
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

```
clear
clc
//Concentration(mol/litre) of components in the
   mixed feed stream is
CAo=1.4;CBo=0.8;CRo=0;
//Volume(litre)
V=6;
//For 75% conversion of B
//From stoichiometry of equation A+2B--->R
CA=1.4-(0.75*0.8)/2;
CB=0.8-(0.75*0.8);
CR=(0.75*0.8)/2;
//From the Given rate equation(mol/litre.min)
rB=2*(12.5*CA*CB*CB-1.5*CR);
//Volumetric flow rate is given by
v=V*rB/(CBo-CB);
printf("\n volumetric flow rate(litre/min) into and
   out of the reactor is %f \n",v)
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

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

Scilab code Exa 5.5 Plug flow reactor volume

```
clear
clc
//Given
//Temperature(kelvin)
T=922;
//Pressure(Pascal)
P=460000;
//Let A=PH3,R=P4,S=H2
FAo=40;//mol/hr
k=10;//(/hr)
R=8.314;
```

```
CAo=P/(R*T);// mol/m3
e=(7-4)/4;
XA=0.8;
//The volume of plug flow reactor is given by
V=FAo*[(1+e)*log(1/(1-XA))-e*XA]/(k*CAo);
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

```
clear
clc
//This is a theorotical Qn
printf("Its a theorotical Question")
```

Chapter 6

Design for Single Reactions

Scilab code Exa 6.1 Operating a number of plug flow reactors

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

Scilab code Exa 6.2 Mixed flow reactor in series

```
clear
```

```
clc
//For single reactor and 90% Conversion
//From fig 6.6
kCot=90;
//For 2 reactor space time is doubled and from fig
kCot=180;
//From graph X=97.4%
X=97.4;
printf("\n Part a")
printf("\n The conversion in percentage is %f \n",X)
//For 90% Conversion & N=2.from graph
kCot=27.5;
//Comparing the reaction rate group for N=1 and N=2, We get
//(V2/v2)/(V1/v1)=27.5/90
//V2=2V1
//Ratio of flow rates
ratio=90*2/27.5;
printf("\n Part b")
printf("\n Treatment rate can be increased by  %f \n",ratio)
```

Scilab code Exa 6.3 Finding the best reactor set up

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

```
for i=1:8
    for j=i:8
        if CA(i)>CA(j)
        temp=CA(i);
        CA(i)=CA(j);
        CA(j)=temp;
        temp1=inv_rA(i);
        inv_rA(i)=inv_rA(j);
        inv_rA(j)=temp1;
        end
    end
end
plot(CA,inv_rA)
xlabel('CA(mmol/m3)');ylabel('-1/rA(m3.min/m mol)');
disp('From the graph,we can see that we should use
   plug flow with recycle')
//From fig
CAin=6.6;//mmol/m3
R=(10-6.6)/(6.6-1);
//V=t*vo=area*vo
V=(10-1)*1.2*vo;
vr=vo*R;
printf("\n Part a")
printf("\n  The vol of reactor is %f",V)
printf("m3 \n The recycle flow rate is %f",vr)
printf("m3/min")
//Part b,from fig
t=(10-1)*10;
t1=(10-2.6)*0.8;
t2=(2.6-1)*10;
//For 1  tank
V=t*vo;
//For  2 tank
V1=t1*vo;
V2=t2*vo;
Vt=V1+V2;
printf("\n Part b")
printf("\n For 1 tank volume is %f",V)
```

```
printf("m3 \n For 2 tank the volume is %f",Vt)
printf("m3")
printf("\n Part c")
disp('We should use mixed flow followed by plug flow
    ')
//For MFR
tm=(10-4)*0.2;
Vm=tm*vo;
//For PFR
tp=5.8;//by graphical integration
Vp=tp*vo;
Vtotal=Vp+Vm;
printf("\n For MFR volume(m3) is %f",Vm)
printf("\n For PFR volume(m3) is %f",Vp)
printf("\n Total volume is %f",Vtotal)
printf("m3")
```

Chapter 7

Design for Parallel Reactions

Scilab code Exa 7.1 Contacting patterns for reactions in parallel

```
clear
clc
//Theorotical Questions
printf("Its a theorotical Question")
```

Scilab code Exa 7.2 Product distribution for parallel reactions

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

```
//But CA=CB so Q(R/A)=CA/(CA+CA^1.5)
//For Plug Flow
//Overall Fractional Yield(Qp) is
CA=CAf;
Qp=(-1/(CAo-CAf))*integrate('1/(1+CA^0.5)','CA',CAo,
    CAf);
CRf=9*Qp;
printf("\n Part a")
printf("\n For Plug Flow")
printf("\n Concentration of R(mol/litre) in the
    product stream is %f \n",CRf)
//Mixed Flow
//Overall Fractional Yield(Qm) is
Qm=CA/(CA+CA^1.5);
CRf=9*Qm;
printf("\n Part b")
printf("\n For Mixed Flow")
printf("\n Concentration of R(mol/litre) in the
    product stream is %f \n",CRf)
//Plug flow A,Mixed flow B
CAo=19;CB=1;
Q=-1/(CAo-CAf)*integrate('CA/(CA+CB^1.5)','CA',CAo,
    CAf);
CRf=9*Q;
printf("\n Part c")
printf("\n For Plug flow A,Mixed flow B")
printf("\n Concentration of R(mol/litre) in the
    product stream is %f \n",CRf)
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

```
clear
```

```
clc
CAo=2;
//Since S is the desired Product
//Q(S/A)=2CA/(1+CA)^2
//Part a
//Csf=(CAo-CA)*2*CA/(1+CA)^2
//on differentiating this to get max Csf,we get max value at
CA=0.5;
Csf=(CAo-CA)*2*CA/(1+CA)^2;
printf("\n Part a")
printf("\n For Mixed Flow Reactor")
printf("\n Maximum expected Cs is %f",Csf)
//For Plug Flow Reactor
//Production of s is max at 100% Conversion of A
CAf=0;
Csf=-1*integrate('2*CA/(1+CA)^2','CA',CAo,CAf);
printf("\n Part b")
printf("\n For Plug Flow")
printf("\n Maximum expected concentration of S is %f \n",Csf)
//Part C
//Since no reactant leaves the system unconverted, what is important is to operate at condition of highest fractional yield
//ie. at CA=1 where Q(S/A)=0.5
CA=1;
Csf=(CAo-CA)*2*CA/(1+CA)^2;
printf("Part c")
printf("\n For MFR with separation and recycle" )
printf("\n Concentration of Csf is %f",Csf)
```

Scilab code Exa 7.4 Best operating conditions for parallel reactions

```
clear
```

```
clc
//Mixed flow followed by plug flow would be best
//From ex 7.3
//For mixed flow
CAo=2;CA=1;Q=0.5;
Cs1=Q*(CAo-CA);
//For plug flow
Cs2=-1*integrate('2*CA/(1+CA)^2','CA',1,0);
//Total amount of CS formed is
Cs=Cs1+Cs2;
printf("Mixed flow followed by plug flow would be
    best")
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

```
clear
clc
//Theorotical Questions
printf("Its a theorotical Question")
```

Scilab code Exa 8.2 Kinetics of series parallel reaction

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

Scilab code Exa 8.3 Evaluate the kinetics from a batch experiment

```
clear
clc
CAo=185;CA=100;t=30;
//As A disappears by 1st Order kinetics
//ln(CAo/CA)=K123t
K123=log(CAo/CA)/t;
//From the initial rate of formation of R
//dCR/dt(m1)=k2*CAo
m1=2;
k2=m1/CAo;
////From the initial rate of formation of R
m2=1.3;
k1=m2/CAo;
k3=K123-k1-k2;
//Looking at the maxima of S and T curves
//For S,CSmax/CAo=(k1/k123)*(k123/k4)^(k4/(k4-k123))
//trial and error
for k4=0.0001:0.0001:0.1
    Csmax=CAo*(k1/K123)*((K123/k4)^(k4/(k4-K123)));
    if  Csmax>31.8 & Csmax<32.2
        break
    end
end
//similarly for T
for k5=0.001:0.0001:0.02
    Ctmax=CAo*(k3/K123)*((K123/k5)^(k5/(k5-K123)));
    if Ctmax>9.95 & Ctmax<10.08
        break
    end
end
printf("\n The rate constants are")
printf("\n k1= %f",k1)
printf("\n k2= %f",k2)
printf("\n k3= %f",k3)
printf("\n k4= %f",k4)
printf("\n k5= %f",k5)
```

Chapter 9

Temperature and Pressure Effects

Scilab code Exa 9.1 AHr AT VARIOUS TEMPERATURES

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

Scilab code Exa 9.2 EQUILIBRIUM CONVERSION AT DIFFERENT TEMPERATURES

```
clear
clc
//Standard heat of reaction(J/mol) and Gibbs free
   energy(J/mol)
Ho=-75300;Go=-14130;
R=8.3214;T1=298;
//With all specific heais alike ,dCp=0
Hr=-Ho;
K298=exp(-Go/(R*T1));
//Taking different values of T
T1=[2;15;25;35;45;55;65;75;85;95];//degree celcius
T=[278;288;298;308;318;328;338;348;358;368];//kelvin
for i=1:10
K=K298*exp((Hr/R)*((1/T(i))-(1/298)));
XAe(i)=K/(K+1);
end
plot(T1,XAe)
xlabel('Temperature(C)')
ylabel('XAe')
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

```
clear
clc
//At 338 k
XA=0.581;
t=1;//min
//From ex 9.2 at 65 degree celcius
XAe=0.89;
```

```
//For a batch reactor ,k1t/XAe=−ln(1−XA/Xae)
k1_338=-(XAe/t)*log(1-(XA/XAe));
//At 25 degree celcius
XAe1=0.993;
T1=338;T2=298;
R=8.314;
//At 298 k
XA1=0.6;
t1=10;//min
k1_298=-(XAe1/t1)*log(1-(XA1/XAe1));
E1=(R*log(k1_338/k1_298))*(T1*T2)/(T1-T2)
ko=k1_338/(exp(-E1/(R*T1)))
//k1=ko*exp(−E1/RT)
//k2=k1/k
printf("\n The rate constants are k=exp[(75300/RT)
    −24.7] min−1")
printf("\n k1=exp[17.2−(48900/RT)] min−1")
printf("\n k2=exp[41.9−(123800/RT)] min−1 ")
```

Scilab code Exa 9.4 PERFORMANCE FOR THE OPTIMAL TEMPERATURE PROGRESSION

```
clear
clc
CAo=4;//mol/litre
FAo=1000;//mol/min
//Drawing locus of max rates on conversion−temp
    graph
//tgen drawing optimum path for this system
//integrating graphicaaly ,we ger
A=0.405;//litre/mol.min
t=CAo*A;
V=FAo*A;
printf("\n Part a")
printf("\n The space time needed is %f",t)
```

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

Scilab code Exa 9.5 OPTIMUM MIXED FLOW REACTOR PERFORMANCE

```
clear
clc
//Concentration of A(mol/litre)
CAo=4;
//Flow rate of A(mol/min)
FAo=1000;
XA=0.8;
Cp=250;//cal/molA.K
Hr=18000;//cal/molA
//Using Xa vs T chart of fig 9.3 at 80% conversion
//Reaction Rate has the value 0.4 mol/min.litre
rA=0.4;
//From the performance eqn for mixed flow,Volume(l) is
V=FAo*XA/rA;
printf("\n Part a")
printf("\n The size of reactor(litres) needed is %f",V)
slope=Cp/Hr;
//Using graph
Qab1=Cp*20;//cal/molA
Qab=Qab1*1000;//cal/min
Qab=Qab*0.000070;//KW
printf("\n Part b")
printf("\n Heat Duty(KW) of precooler is %f",Qab)
Qce1=Cp*37;//cal/molA fed
Qce=Qce1*1000;//cal/min
Qce=Qce*0.000070;//KW
printf("\n Heat Duty(KW) of postcooler is %f",Qce)
```

Scilab code Exa 9.6 ADIABATIC PLUG FLOW REACTOR PERFORMANCE

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

Scilab code Exa 9.7 ADIABATIC PLUG FLOW REACTOR WITH RECYCLE I Repeat

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

Chapter 10

Choosing the Right Kind of Reactor

Scilab code Exa 10.1 THE TRAMBOUZE REACTIONS

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

Scilab code Exa 10.2 TEMPERATURE PROGRESSION FOR MULTIPLE REACTIONS

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

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

```
end
plot(T,E)
xlabel('time(min)')
ylabel('E(min^-1)')
title('Exit age distribution E vs time')
```

Scilab code Exa 11.2 FINDING THE E CURVE FOR LIQUID FLOWING THROUGH A VESSEL

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

```
Vl=t*v;
//Fraction of liquid
f=Vl/V;
printf("\n Part b")
printf("\n Fraction of liquid is %f",f)
//E=Cpulse/M/v
printf("\n Part c")
printf("\n The E curve is 1.5C")
printf("\n Part d")
printf("\n The vessel has  a strong recirculation of
    liquid ,probably induced by the rising bubbles")
```

Scilab code Exa 11.3 CONVOLUTION

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

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

Scilab code Exa 11.4 CONVERSION IN REACTORS HAVING NON IDEAL FLOW

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

Scilab code Exa 11.5 REACTION OF A MACROFLUID

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

```
//CA/CAo=1/(1+kCAo*t)
to=1;t1=3;
E=0.5;
//Using eqn 13
XA_avg=1-(E*integrate('1/(1+t)','t',to,t1));
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

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

Scilab code Exa 12.2 MISBEHAVING REACTOR

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

Chapter 13

The Dispersion Model

Scilab code Exa 13.1 DluL FROM A C CURVE

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

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

Scilab code Exa 13.2 DuL FROM AN F CURVE

```
clear
clc
//length of column(mm)
l=1219;
//Velocity(mm/s)
u=0.0067;
//Using the probability graph
//16th percentile point fall at
t1=178550;
//84th percentile point fall at
t2=187750;
//standard deviation
sigma=(t2-t1)/2;
t=l/u;
sigma_theta=sigma/t;
//Vessel dispersion number
d=sigma_theta^2/2;
printf("\n The vessel dispersion number is %f",d)
```

Scilab code Exa 13.3 DuL FROM A ONE SHOT INPUT

```
clear
clc
```

```
//Bed voidage
v=0.4;
//Superficial velocity of fluid(cm/s)
u=1.2;
l=90;//length(cm)
//Variance(sec^2) of output signals
sigma1_sqr=39;sigma2_sqr=64;
dsigma_sqr=sigma2_sqr-sigma1_sqr;
//In dimensionless form
t=l*v/u;
sigmatheta_sqr=dsigma_sqr/t^2;
//Dispersion number
d=sigmatheta_sqr/2;
printf("\n The vessel dispersion number is %f",d)
```

Scilab code Exa 13.4 CONVERSION FROM THE DISPERSION MODEL

```
clear
clc
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

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

Scilab code Exa 14.2 A FABLE ON RIVER POLLUTION

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

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

Scilab code Exa 14.3 F LOW MODELS FROM RTD CURVES

```
clear
clc
vo=1;
t1=1/6;
t2=1;
t3=11/6;
w=1/10;
//Ratio of areas of the first 2 peaks
A2_by_A1=0.5;
R=A2_by_A1/(1-A2_by_A1);
//From the location of 1st peak
V1=(R+1)*vo*t1;
//From the time between peaks
V2=(R*vo)*((t2-t1)-(t1));
//From fig 14.3
N=1+(2*(t1/w))^2;
printf("\n The reflux ratio is %f",R)
printf("\n The volume of 1st tank is %f", V1)
printf("\n The volume of 2nd tank is %f",V2)
printf("\n The number of tanks are %f ",N)
```

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

```
clear
clc
```

```
//from fig E14.4a
t2=280;t1=220;
sigma1_sqr=100;sigma2_sqr=1000;
dt=t2-t1;
dsigma_sqr=sigma2_sqr-sigma1_sqr;
N=dt^2/dsigma_sqr;
for t=1:200
//For N tank in series
E(t)=((t^(N-1))*(N^N)*exp(-t*N/dt))/((factorial(N-1))*(dt^N));
end
for i=1:200
    t(i)=i;
end
plot(t,E)
xlabel('time(sec)')
ylabel('E(sec^-1)')
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

```
clear
clc
Co=1;k=1;t=1;//given
//Scheme A
//For mixed flow reactor
//t=(Co-C1)/KC1^2
C1=(-1+sqrt(1-4*t*(-Co)))/2*t;
//For the plug flow reactor
//t=1/k(1/C2-1/C1)
C2=C1/(1+k*t*C1);
printf("\n Conversion for flow scheme A is %f",C2)
//Scheme B
//For plug flow
C3=Co/(1+k*t*Co);
//For mixed flow reactor
C4=(-1+sqrt(1-4*t*(-C3)))/2*t;
printf("\n Conversion for flow scheme B is %f",C4)
//Scheme C,D,E
```

```
//Using exit age distribution fn for 2 equal plug-
    mixed flow reactor system,using fig 12.1
t_bar=2;
in=1000;
C5=integrate('(2/t_bar)*(exp(1-2*t/t_bar))/(1+Co*k*t
    )','t',t_bar/2,in);
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

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

Scilab code Exa 17.2 AEROBIC FERMENTATION

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

Scilab code Exa 17.3 OVERALL RATE FOR A LINEAR PROCESS

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

Scilab code Exa 17.4 OVERALL RATE FOR A NONLINEAR PROCESS

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

Chapter 18

Solid Catalyzed Reactions

Scilab code Exa 18.1 SEARCH OF THE RATE CONTROLLING MECHANISM

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

```
if ratio<0.01
    printf("\n Resistance to mass transport to film
       should not influence rate of reaction")
else
      printf("\n Resistance to mass transport to
         film should influence rate of reaction")
end
printf("\n Part b")

Mw=rA_obs*(L^2)/(De*CAg);
printf("\n Mw= %f",Mw)
if Mw>4
  printf("\n Pore diffusion is influencing and hence
      strong pore diffusion")
else
      printf("\n Pore diffusion is  not influencing
         and hence weak pore diffuusion")
end
//Temp variation within pellet
dt_max_pellet=De*(CAg-0)*(-Hr)/Keff;
//Temp variation Across the gas film
dt_max_film=L*rA_obs*(-Hr)/h;
printf("\n Part c")
printf("\n dTmax,pellet is %f",dt_max_pellet)
printf(" degree C \n dTmax,film is %f",dt_max_film)
printf(" degree C")
if dt_max_pellet<1
    printf("\n Pellet is close to uniform in
       temperature")
else
    printf("\n There is a variation in temp within
       pellet")
    end
    if dt_max_film<1
    printf("\n Film is close to uniform in
       temperature")
else
    printf("\n There is a variation in temp within
```

```
    Film")

end
```

Scilab code Exa 18.2 THE RATE EQUATION FROM A DIFFERENTIAL REACTOR

```
clear
clc
//Pressure(atm)
PAo=3.2;
R=0.082;//litre.atm/mol.k
T=390;//k
v=20;//litre/hr
W=0.01;///kg
CA_in=[0.1;0.08;0.06;0.04];
CA_out=[0.084;0.07;0.055;0.038];
CAo=PAo/(R*T);
FAo=CAo*v;
eA=3;
for i=1:4
XA_in(i)=(1-CA_in(i)/CAo)/(1+eA*CA_in(i)/CAo);
XA_out(i)=(1-CA_out(i)/CAo)/(1+eA*CA_out(i)/CAo);
dXA(i)=XA_out(i)-XA_in(i);
rA(i)=dXA(i)/(W/FAo);
CA_avg(i)=(CA_in(i)+CA_out(i))/2;
end
plot(CA_avg,rA)
xlabel('CA(mol/litre)')
ylabel('-rA(mol/hr.kg)')
coeff1=regress(CA_avg,rA)
k=coeff1(2)
printf("\n The rate of reaction(mol/hr.kg) is %f",k)
printf("CA")
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

```
clear
clc
CAo=0.1;//mol/litre
FAo=2;//mol/hr
eA=3;
CA=[0.074;0.06;0.044;0.029];//mol/litre
W=[0.02;0.04;0.08;0.16];//kg
//Gussing 1st order,plug flow rxn
//(1+eA)*log(1/(1-XA))-eA*XA=k*(CAo*W/FAo)
for i=1:4
XA(i)=(CAo-CA(i))/(CAo+eA*CA(i));
y(i)=(1+eA)*log(1/(1-XA(i)))-eA*XA(i);
x(i)=CAo*W(i)/FAo;
W_by_FAo(i)=W(i)/FAo;
CAout_by_CAo(i)=CA(i)/CAo;
XA1(i)=(1-CAout_by_CAo(i))/(1+eA*CAout_by_CAo(i));
end
plot(x,y)
coeff3=regress(x,y);
xlabel('CAoW/FAo'),ylabel('4ln(1/1-XA)-3XA')
k=coeff3(2);
printf("\n Part a,using integral method of analysis")
printf("\n The rate of reaction(mol/litre) is %f",k)
printf("CA")
//Part b
//plotting W_by_FAo vs XA1,the calculating rA=dXA/d(W/FAo) for last 3 points,we get
rA=[5.62;4.13;2.715];
```

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

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

```
clear
clc
XA=0.35;
FAo=2000;//mol/hr
eA=3;k=96;
CAo=0.1;
W=((1+eA)*log(1/(1-XA))-eA*XA)*(FAo/(k*CAo));
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

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

```
inv_rA(i)=1/rA(i);
end
//W=FAo*integral(dXA/-rA) from 0 to 0.35
//Using Trapezoidal rule to find area,XA must be in
    increasing order
//Sorting XA and accordingly inv_rA
for i=1:4
    small=XA(i);
    for j=i:4
        next=XA(j);
        if small>next
            temp=XA(i);
            XA(i)=XA(j);
            XA(j)=temp;
            temp1=inv_rA(i);
            inv_rA(i)=inv_rA(j);
            inv_rA(j)=temp1;
        end
    end
end
plot(XA,inv_rA)
xlabel('XA');ylabel('-1/rA');
//extending points to include XA=0.35
XA(5)=0.35;inv_rA(5)=0.34;
Area=inttrap(XA,inv_rA);
W=Area*2000;
printf("Amount of catalyst needed(kg) is %f",W)
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

```
clear
clc
```

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

Scilab code Exa 18.7 MASS TRANSFER RESISTANCES

```
clear
clc
printf("Its a theorotical qn")
```

Chapter 19

The Packed Bed Catalytic Reactor

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

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

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

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

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

```
//Using method of maximization of rectangles
area1=0.66*3.6;
area2=(0.85-0.66)*20;
W1=FAo*area1;
W2=FAo*area2;
printf("\n The weight of catalyst needed for 1st bed
    is %f",W1)
printf("kg \n The weight of catalyst needed for 2
   ndbed is %f",W2)
printf("kg")
//Heat exchange
//For the first reactor
//To go to 66% conversion at 820 degree C,the amount
    of heat needed per mol of A is
Q=(820-300)*Cp+0.66*(-Hr);
//For 100 mol/s
Q1= FAo*Q/10^6;//MW
printf("\n The amount of heat exchanged for 1st
   reactor is %f",Q1)
printf("MW")
//For 2nd reactor
//To go from XA=0.66 at 820 k to XA=0.85 at 750 k
Q2=FAo*((750-820)*Cp+(0.85-0.66)*(-Hr));
Q2=Q2/10^6;
printf("\n The amount of heat exchanged for 2nd
   reactor is %f",Q2)
printf("MW")
//For the exchanger needed to cool the exit stream
   from 750 k to 300 k
Q3=FAo*Cp*(300-750);
Q3=Q3/10^6;//MW
printf("\n The amount of heat exchanged for
   exchanger is %f",Q3)
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

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

```
ub=uo-umf+ubr;
delta=uo/ub;
ef=1-(1-emf)*(1-delta);
Kbc=4.5*(umf/db)+5.85*(D^0.5)*(g^0.25)/(db^1.25);
Kce=6.77*sqrt(emf*D*ubr/db^3);
fb=0.001;
fc=delta*(1-emf)*((3*umf/emf)/(ubr-umf/emf)+alpha);
fe=(1-emf)*(1-delta)-fc-fb;
ft=fb+fe+fc;
A=3.14*d*d/4;
Hbfb=W/((density*A)*(1-ef));
XA=1-inv(exp(fb*k+(1/((1/(delta*Kbc))+1/((fc*k)
    +(1/((1/(delta*Kce))+(1/(fe*k)))))))*(Hbfb*ft/uo)
    /ft));
XA1=100*XA;//in percentage
printf("\n Part a")
printf("\n Conversion of reactant is %f ",XA1)
CA_avg=CAo*XA*vo*density/(k*W);
printf("\n Part b")
printf("\n The proper mean concentration(mol/m3) of
    A seen by solid is %f",CA_avg)
XA1=1-inv(exp(k*ft*Hbfb/uo));
printf("\n Part c")
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

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

```
kd=coeff(2);
k=exp(coeff(1))/t1;
L=d/6;
Mt=L*sqrt(k*density_s/De);
//Assuming Runs were made in regime of strong resistance to pore diffusion
k1=((exp(coeff(1)))^2)*(L^2)*density_s/(t1*t1*De);
kd1=-2*coeff(2);
Mt=L*sqrt(k1*density_s/De);
printf("\n Rate equation(mol/kg.s) in diffusion free regime with deactivation is %f ",k1)
printf("CA*a with \n -da/dt(hr-1) is %f",kd1)
printf("a")
//In strong pore diffusion
k2=k1*sqrt(De/(k1*density_s));
printf("\n Rate equation(mol/kg.s) in strong pore diffusion resistance regime with deactivation is %f ",k2)
printf("CA*a^0.5/L with \n -da/dt(hr-1) is %f",kd1)
printf("a")
```

Scilab code Exa 21.2 DEACTIVATION IN A PACKED BED REACTOR

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

```
 //Part a
a(i)=1-(8.3125*10^-3)*t;
XA(i)=(tau^2)*a(i)/(1+(tau^2)*a(i));
//Part b
a1(i)=exp(-0.05*t);
XA1(i)=(tau^2)*a1(i)/(1+(tau^2)*a1(i));
//Part c
a2(i)=1/(1+3.325*t);
XA2(i)=(tau^2)*a2(i)/(1+(tau^2)*a2(i));
//Part d
a3(i)=1/(sqrt(1+1333*t));
XA3(i)=(tau^2)*a3(i)/(1+(tau^2)*a3(i));
end
t=[0:5:120];
plot(t,XA,t,XA1,t,XA2,t,XA3)
xlabel('Time(days)')
ylabel('XA')
legend('Zero Order','1st Order','2nd Order','3rd Order');
XA_avg=(1/120)*integrate('(100*(1-(8.3125*10^-3)*t))/(1+100*(1-(8.3125*10^-3)*t))','t',0,120);
XA1_avg=(1/120)*integrate('(100*exp(-0.05*t))/(1+100*exp(-0.05*t))','t',0,120);
XA2_avg=(1/120)*integrate('(100*(1/(1+3.325*t)))/(1+100*(1/(1+3.325*t)))','t',0,120);
XA3_avg=(1/120)*integrate('(100*1/(sqrt(1+1333*t)))/(1+100*(1/sqrt(1+1333*t)))','t',0,120);
printf("\n for d=0,the mean conversion is %f",XA_avg)
printf("\n for d=1,the mean conversion is %f",XA1_avg)
printf("\n for d=2,the mean conversion is %f",XA2_avg)
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

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

```
kai_overall=0.02;
kac_ac=0.05;
f=0.6;
//For a half-order reaction
Mt=L*sqrt((n+1)*(k*d_solid*(CA)^(n-1))/(2*De));
E=1/Mt;
rA=(1/((1/(kai_overall))+(1/(kac_ac))+(1/(k*b*(CA^(n
    -1))*E*f*d_solid))))*(PA/HA);
//From Material Balance
XB=b*rA*Vr/FBo;
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

```
clear
clc
PA=14.6*101325;//Pa
HA=148000;
Vr=2;
Vl=Vr;
b=1;
fs=0.0055;
k=5*10^-5;//m6l/kg.molcat.s
dp=5*10^-5;//mcat
kac=4.4*10^-4;kai=0.277;//m3l/m3.r.s
density=1450;//kg/m3
De=5*10^-10;//m3l/mcat.s
L=dp/6;//for spherical particle
CA=PA/HA;
X=0.9;
CBo=2500;//mol/m3.l
CB=CBo*(1-X);
ac=6*fs/dp;;
K=kac*ac;
```

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

Chapter 23

Fluid Fluid Reactions Kinetics

Scilab code Exa 23.1 FINDING THE RATE OF A GL REACTION

```
clear
clc
k=10^6;
Kag_a=0.01;fl=0.98;
Kal=1;
HA=10^5;
DAl=10^-6;
DBl=DAl;
PA=5*10^3;//Pa
CB=100;//mol/m3
b=2;
a=20;//m2/m3
Mh=sqrt(DAl*k*CB*CB)/Kal;
Ei=1+(DBl*CB*HA/(b*DAl*PA));
E=100;
printf("\n Part a")
res_total=(((1/(Kag_a))+(HA/(Kal*a*E))+(HA/(k*CB*CB*fl))));//Total Resistance
f_gas=(1/(Kag_a))/res_total;//fraction of resistance in gas film
f_liq=(HA/(Kal*a*E))/res_total;//fraction of
```

```
    resistance in liquid film
printf("\n Fraction of the resistance in the gas
    film is %f",f_gas)
printf("\n Fraction of the resistance in the liquid
    film is %f",f_liq)
printf("\n Part b")
printf("\n The reaction zone is in the liquid film")
printf("\n Part c")
if Ei>5*Mh
    printf("\n We have pseudo 1st order reaction in
        the film")
end
//From fig 23.4

rA=PA/(((1/(Kag_a))+(HA/(Kal*a*E))+(HA/(k*CB*CB*fl))
    ));
printf("\n Part d")
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

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

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

Scilab code Exa 24.2 TOWERS FOR HIGH CONCENTRATION OF LIQUID REACTANT

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

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

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

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

Scilab code Exa 24.4 TOWERS FOR INTERMEDIATE CONCENTRATIONS OF LIQUID REACTANT

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

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

```
clear
clc
Fg=10^5;
P=10^5;
Fg_by_Acs=10^5;//(Fg/Acs)
PA1=20;PA2=100;
```

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

Scilab code Exa 24.6 REACTION OF A BATCH OF LIQUID

```
clear
clc
kag_a=0.72;
kal_a=144;
HA=1000;
Fg=9000;//mol/hr
fl=0.9;b=1;
Vr=1.62;//m3
DA=3.6*10^-6;//m2/hr
a=100;//m2/m3
k=2.6*10^5;//m3/mol.hr
DB=DA;
P=10^5;PA=1000;//Pa
kal=kal_a/a;
//At the start
CBo=555.6;
Mh=(sqrt(DB*k*CBo))/kal;
//Min value of EAi
Ei=1+(CBo*HA/PA);
if Ei>Mh
    E=Mh;
end
rA1=PA/((P*Vr/Fg)+(1/kag_a)+(HA/(kal_a*E))+(HA/(k*fl
```

```
    *CBo)));
//At the end
CBf=55.6;
Mh=(sqrt(DB*k*CBf))/kal;
//Min value of EAi
Ei=1+(CBf*HA/PA);
if Ei>Mh
    E=Mh;
end
rA2=PA/((P*Vr/Fg)+(1/kag_a)+(HA/(kal_a*E))+(HA/(k*fl
    *CBf)));
//Average rate of reaction
rA_avg=(rA1+rA2)/2;
t=(fl/b)*integrate('1/rA_avg','CB',CBf,CBo);
printf("\n Part a")
printf("\n The run time needed is %f",t)
printf("hr")
//The min time required is
tmin=Vr*(CBo-CBf)/(Fg*(PA/(P-PA)));
printf("\n The minimum time required is %f",tmin)
printf("hr")
//Fraction of reactant which passes through the tank
    unreacted is
f=(t-tmin)/tmin;
printf("\n Part b")
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

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

```
end
f_converted=1-sum1;
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

```
clear
clc
t_avg=60;t=20;//min
//For chemical rxn controlling , t =kR
unconverted=((1/4)*(t/t_avg))-((1/20)*(t/t_avg)^2)
    +((1/120)*(t/t_avg)^3);
//For ash layer diffusion controlling ,t=k1R^2
unconverted1=((1/5)*(t/t_avg))-((19/420)*(t/t_avg)
    ^2)+((41/4620)*(t/t_avg)^3);
c_avg=(unconverted+unconverted1)/2;
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

```
clear
clc
F=1000;//gm/min
W=10000;//gm
t_avg=W/F;
F_50=300;F_100=400;F_200=300;//gm/min
t_50=5;t_100=10;t_200=20;//min
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));
converted=1-unconverted;
printf("The mean conversion of soild is %f",
   converted)
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

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

Chapter 29

Substrate Limiting Microbial Fermentation

Scilab code Exa 29.1 MIXED REACTORS FOR MONOD KINETICS

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

Scilab code Exa 29.2 PLUG FLOW REACTOR FOR MONOD KINETICS

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

Scilab code Exa 29.3 GLUCOSE FOR E COLI BACTERIA

```
clear
```

```
clc
CAo=6;CM=0.4;//kg/m3
V=1;//m3
k=4;
//From fig 29.5
N=sqrt(1+(CAo/CM));
kt_op=N/(N-1);
C_by_A=0.1;
t_op=kt_op/k;
v_op=V/t_op;
//The feed rate of glucose
FAo=v_op*CAo;
printf("\n The feed rate of glucose is %f",FAo)
printf("kg/hr")
//Max consumption rate of glucose is
XA=N/(N+1);
c_max=FAo*XA;
printf("\n Max consumption rate of glucose is %f ",
    c_max)
printf("kg/hr")
//Max production rate of E.coli is
Cc_op=(C_by_A)*CAo*N/(N+1);
Fcmax=v_op*Cc_op;
printf("\n Max production rate of E.coli is %f",
    Fcmax)
printf("kg/hr")
```

Chapter 30

Product Limiting Microbial Fermentation

Scilab code Exa 30.1 FRUIT FLY COCKTAIL

```
clear
clc
k=sqrt(3);//hr^-1
n=1;
V=30;//m3
CR=0.12;//kgalc/kgsol
density=1000;//kg/m3
//CR in kg/m3
CR=CR*density;
CR_opt=CR/2;
alcohol_per=CR_opt*100/density;//PErcentage of
    alcohol
printf("\n The Percentage of alchol in cocktail is
    %f",alcohol_per)
//From fig 30.4
kt=1;
t=kt/k;
t_opt=2*t;
v_opt=V/t_opt;
```

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