# Scilab Textbook Companion for Chemical Reactor Design by P. Harriott[1]

Created by
Sneha R Iyer
B-Tech Chemical Engineering
Chemical Engineering
SASTRA University ,Thanjavur
College Teacher
NA
Cross-Checked by
Spandana

July 31, 2019

[1] Funded by a grant from the National Mission on Education through ICT, http://spoken-tutorial.org/NMEICT-Intro. This Textbook Companion and Scilab codes written in it can be downloaded from the "Textbook Companion Project" section at the website http://scilab.in

# Book Description

**Title:** Chemical Reactor Design

**Author:** P. Harriott

**Publisher:** CRC Press

**Edition:** 1

**Year:** 2002

**ISBN:** 978-0824708818

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

# Homogeneous Kinetics

**Scilab code Exa 1.4** `Activation energy from packed bed data`

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition
    ) Marcel Dekker,Inc.,USA,pp 436.
//Chapter-1 Ex1.4  Pg No. 23
//Title: Activation energy from packed bed data
//
    ================================================================
clear
clc
clf
// COMMON INPUT
L= [0 1 2 3 4 5 6 9];//Bed length in feet(ft)
T=[330 338 348 361 380 415 447 458 ] //Temperature
    Corresponding the bed length given ( C )
R=1.98587E-3;//Gas constant (kcal/mol K)

//CALCLATION (Ex1.4.a)
```

```
//Basis is 1mol of feed A(Furfural) X moles reacted to form Furfuran and CO
x=(T-330)./130;//Conversion based on fractional temperature rise
n=length (T);//6 moles of steam per mole of Furfural is used to decrease temperature rise in the bed
P_mol=x+7;//Total No. of moles in product stream
for i=1:(n-1)
    T_avg(i)= (T(i)+T(i+1))/2
    P_molavg(i)= (P_mol(i)+P_mol(i+1))/2
    delta_L(i)=L(i+1)-L(i)
    k_1(i)=((P_molavg(i))/delta_L(i))*log((1-x(i))/(1-x(i+1)))
    u1(i)=(1/(T_avg(i)+273.15));
end
v1=(log(k_1));
i=length(u1);
X1=[u1 ones(i,1) ];
result1= X1\v1;
k_1_dash=exp(result1(2,1));
E1=(-R)*(result1(1,1));

//OUTPUT (Ex1.4.a)
//Console Output
mprintf('\n OUTPUT Ex1.4.a');
mprintf('\n
==========================================================================
n')
mprintf('L \t \t T \t\t x \t\t T_average \t(7+x)ave \tk_1')
mprintf('\n(ft) \t \t ( C ) \t\t   \t\t ( C ) \t   ')
mprintf('\n
==========================================================================
')
for i=1:n-1
mprintf('\n%f \t %f \t %f ',L(i+1),T(i+1),x(i+1))
mprintf('\t %f \t %f \t %f',T_avg(i),P_molavg(i),k_1(i))
```

```
end
mprintf('\n\nThe activation energy from the slope = %f kcal/mol',E1 );
//==================================================================


//Title: II Order Reaction
//==================================================================

//CALCULATION (Ex 1.4.b)
for i=1:(n-1)
    T_avg(i)= (T(i)+T(i+1))/2
    P_molavg(i)= (P_mol(i)+P_mol(i+1))/2
    delta_L(i)=L(i+1)-L(i)
    k_2(i)=((P_molavg(i))/delta_L(i))*((x(i+1)-x(i))/((1-x(i+1))*(1-x(i))))
    u2(i)=(1/(T_avg(i)+273.15));
end
v2=(log(k_2));
plot(u1.*1000,v1,'o',u2.*1000,v2,'*');
xlabel("1000/T (K^-1)");
ylabel("ln k_1 or ln k_2");
xtitle("ln k vs 1000/T ");
legend('ln k_1','ln k_2');
j=length(u2);
X2=[u2 ones(j,1) ];
result2= X2\v2;
k_2_dash=exp(result2(2,1));
E2=(-R)*(result2(1,1));

//OUTPUT (Ex 1.4.b)
mprintf('\n OUTPUT Ex1.4.b');
mprintf('\n==================================================================n')
mprintf('L \t \t T \t\t x \t\t T_average \t(7+x)ave \tk_2')
mprintf('\n(ft) \t \t ( C ) \t\t  \t\t ( C ) \t  ')
mprintf('\n============================================================
')
for i=1:n-1
mprintf('\n%f \t %f \t %f ',L(i+1),T(i+1),x(i+1))
mprintf('\t %f \t %f \t %f',T_avg(i),P_molavg(i),k_2(i))
end
mprintf('\n\nThe activation energy from the slope = %f kcal/mol',E2 );

//FILE OUTPUT
fid= mopen('.\Chapter1-Ex4-Output.txt','w');
mfprintf(fid,'\n OUTPUT Ex1.4.a');
mfprintf(fid,'\n============================================================
n')
mfprintf(fid,'L \t \t T \t\t x \t\t T_average \t(7+x)ave \tk_1')
mfprintf(fid,'\n(ft) \t \t ( C ) \t\t  \t\t ( C ) \t  ')
mfprintf(fid,'\n============================================================
')
for i=1:n-1
mfprintf(fid,'\n%f \t %f \t %f ',L(i+1),T(i+1),x(i+1))
mfprintf(fid,'\t %f \t %f \t %f',T_avg(i),P_molavg(i),k_1(i))
end
mfprintf(fid,'\n\nThe activation energy from the slope =%f kcal/mol',E1 );
mfprintf(fid,'\n\n============================================================
n')
```

```
mfprintf(fid,'\n OUTPUT Ex1.4.b');
mfprintf(fid,'\n================================================================\n')
mfprintf(fid,'L \t \t T \t\t x \t\t T_average \t(7+x)ave \tk_2')
mfprintf(fid,'\n(ft) \t \t ( C ) \t\t  \t\t ( C ) \t  ')
mfprintf(fid,'\n================================================================')
for i=1:n-1
mfprintf(fid,'\n%f \t %f \t %f ',L(i+1),T(i+1),x(i+1))
mfprintf(fid,'\t %f \t %f \t %f',T_avg(i),P_molavg(i),k_2(i))
end
mfprintf(fid,'\n\nThe activation energy from the slope =%f kcal/mol',E2 );
close;

//==========================================================END OF PROGRAM==========================================================
//Disclaimer (Ex1.4.a):The last value of tavg and k_1  corresponding to L=9 in Table 1.6 (Pg No. 25)of the textbook is a misprint.
// The value should be 452.5 and 4.955476 respectively instead of 455 and 18.2 as printed in the textbook.
//Hence there is a change in the activation energy obtained from the code
// The answer obtained is 21.3935 kcal/mol instead of 27 kcal/mol as reported in the textbook.
//Figure 1.8 is a plot between ln k_1 vs 1000/T instead of k_1 vs 1000/T as stated in the solution of Ex1.4.a
```

```
//
//Disclaimer (Ex1.4.b): There is a discrepancy between the computed value of activation energy and value reported in textbook
// Error could have been on similar lines as reported for example Ex.1.4.a
// Further, intermeidate values for Ex.1.4.b is not available/ reported in textbook and hence could not be compared.
//Figure 1.8 is a plot between ln k_2 vs 1000/T instead of k_2 vs 1000/T as stated in the solution of Ex1.4.b
```

**Scilab code Exa 1.5** Methods to determine km and vm

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc.,USA,pp 436.
//Chapter-1 Ex1.5 Pg No. 29
//Title: Methods to determine km and vm
//
clear
clc
clf
//INPUT
S=[2;5;10;15]*10^(-3);//Concentration of substrate [HCO3]
r_reciprocal=[95;45;29;25]*10^(3);//Reciprocal rates
```

```
    (L-sec/mol)

//CALCULATION
//Plot 1 refer equation 1.24 Pg No.29
x1=(S).^(-1);
y1=r_reciprocal;
scf(0)
plot(x1,y1*10^(-3),'RED');
xlabel("1/[S]");
ylabel("(1/r)*10^-3");
xtitle("1/r versus 1/S");
p=length(x1);
X_1=[x1 ones(p,1)];
R1=X_1\y1;
slope(1)=R1(1,1);
intercept(1)=R1(2,1);
v_m(1)=(1/(intercept(1)));//Maximum Reaction Rate(
   mol/L-sec)
k_m(1)=slope(1)*v_m(1);//Michaelis-Menton constant

//Plot 2 refer equation 1.25 Pg No.29
x2=S;
y2=S.*r_reciprocal;
scf(1)
plot(x2*10^(3),y2);
xlabel("(S)*10^3");
ylabel("(S)/r");
xtitle("(S)/r versus (S)");
q=length(x2);
X_2=[x2 ones(q,1)];
R2=X_2\y2;
slope(2)=R2(1,1);
intercept(2)=R2(2,1);
v_m(2)=1/(slope(2));//Maximum Reaction Rate (mol/L-
   sec)
k_m(2)=intercept(2)/(slope(2));//Michaelis-Menton
   constant

```

```

//OUTPUT
mprintf('\n================================================================================');
mprintf('\n     \t\tMethod_1\tMethod_2');
mprintf('\n================================================================================');
i=1
    mprintf('\n  Slope     \t%f\t%f',slope(i),slope(i+1));
    mprintf('\n  Intercept  \t%f\t%f',intercept(i),intercept(i+1));
    mprintf('\n  Km (M)       \t%f\t%f',k_m(i),k_m(i+1));
    mprintf('\n  Vm(mol/L-sec) %f\t%f',v_m(i),v_m(i+1));

//FILE OUTPUT
fid= mopen('.\Chapter1-Ex5-Output.txt','w');
mfprintf(fid,'\n================================================================================');
mfprintf(fid,'\n     \t\tMethod_1\tMethod_2');
mfprintf(fid,'\n================================================================================');
i=1
    mfprintf(fid,'\n  Slope     \t%f\t%f',slope(i),slope(i+1));
    mfprintf(fid,'\n  Intercept  \t%f\t%f',intercept(i),intercept(i+1));
    mfprintf(fid,'\n  Km (M)       \t%f\t%f',k_m(i),k_m(i+1));
    mfprintf(fid,'\n  Vm(mol/L-sec) %f\t%f',v_m(i),v_m(i+1));
mclose(fid);
```

```

//=============================================END OF PROGRAM===========================
//Disclaimer: Least Square method is used to find the slope and intercept in this example.
// Hence the values differ from the graphically obtained values of slope and intercept in the textbook.
```

# Chapter 2

# Kinetic Models for Heterogeneous Reactions

**Scilab code Exa 2.1** Effectiveness factor for solid catalyzed reaction

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc. USA,pp 436.
//Chapter-2 Ex2.1 Pg No.52
//Title: Effectiveness factor for solid catalyzed reaction
//================================================================================================
clear
clc
function [coefs]=regress(x,y)
 coefs=[]
  if (type(x) <> 1)|(type(y)<>1) then error(msprintf(gettext(”%s: Wrong type for input arguments: Numerical expected.\n”),”regress”)), end
  lx=length(x)
  if lx<>length(y) then error(msprintf(gettext("%s: Wrong size for both input arguments: same size expected.\n"),"regress")), end
  if lx==0 then error(msprintf(gettext("%s: Wrong size for input argument #%d: Must be > %d.\n"),"regress", 1, 0)), end
  x=matrix(x,lx,1)
  y=matrix(y,lx,1)
  xbar=sum(x)/lx
  ybar=sum(y)/lx
  coefs(2)=sum((x-xbar).*(y-ybar))/sum((x-xbar).^2)
  coefs(1)=ybar-coefs(2)*xbar
endfunction
clf
//INPUT
// Case: I  constant hydrogen pressure: P_H2= 2110 torr
P_B=[70 185 286];// Benzene Pressure (torr)
r_1=1E-3 *[4.27 5.4 6.12];//(mol/hr g) observed rates
P_H2_const=2110;//Constant Hydrogen Pressure (torr)


// Case: II  Constant benzene pressure P_B_const=70 torr
P_H2=[1050 2105 2988];// Hydrogen Pressure (torr)
r_2=1E-3 * [3.81 4.27 4.5];//(mol/hr g) observed rates
P_B_const=70;//Constant Benzene Pressure (torr)

//CALCULATION
// Case: I  constant hydrogen pressure: P_H2= 2110 torr

n=length(P_B)
for i=1:n
    Y_1(i)=(P_B(i)*P_H2_const/r_1(i))^(1/3);
    X_1(i)=P_B(i);
end
coefs_I=regress(X_1',Y_1');
intercept_1=coefs_I(1)
slope_1=coefs_I(2)

// Case: II  Constant benzene pressure P_B_const=70 torr
m=length(P_H2)
for i=1:n
    Y_2(i)=(P_B_const*P_H2(i)/r_2(i))^(1/3);
    X_2(i)=(P_H2(i))^0.5;
end
coefs_II=regress(X_2',Y_2');
intercept_2=coefs_II(1);
slope_2=coefs_II(2);
coef_1=(intercept_1)^0.5;
coef_2=(slope_1*slope_2)^(1/2)*(slope_1/slope_2)*intercept_1;

function y=funct1(K_H2)
    y=coef_2*K_H2^0.5-coef_1*K_H2^(4/3)-1
endfunction

[K_H2_res]=fsolve(0,funct1);

K_B=K_H2_res^(4/3)*(slope_1/slope_2);

k=(0.635)^(-1/3)*K_B^2/K_H2_res;
scf(0)
plot(X_1,Y_1,'-*-')
xtitle('Benzene Hydrogenation(a)Variable benzene pressure')
xlabel("P_B (torr)");
ylabel("(P_H2 P_B/10^3 r)^(1/3)");
legend('T=67.6  C ');

scf(1)
```

```
plot(X_2,Y_2,'-*-')
xtitle('Benzene Hydrogenation(b)Variable hydrogen pressure')
xlabel("P_H2 (torr)");
ylabel("(P_H2 P_B/10^3 r)^(1/3)");
legend('T=67.6  C ');

//OUTPUT
mprintf('\n Solving for the three parameters gives');
mprintf('\n K_H2 = %f torr^-1',K_H2_res);
mprintf('\n K_B = %f torr^-1',K_B);
mprintf('\n k = %E ',k);

//FILE OUTPUT
fid= mopen('.\Chapter2-Ex1-Output.txt','w');
mfprintf(fid,'\n Solving for the three parameters gives');
mfprintf(fid,'\n K_H2 = %f torr^-1',K_H2_res);
mfprintf(fid,'\n K_B = %f torr^-1',K_B);
mfprintf(fid,'\n k = %E ',k);
mclose(fid);

//==================================================================

//Disclaimer: Page 53 There is a typo in the equation for Y obtained for Model case I: Constant hydrogen pressure and variable benzene pressure formulation
// From Fig 2.7(a), It is evident that for P_H2 = 2110 torr, three experimental points are considered for linear regression. However, from table 2.1, only two points corresponds to P_H2 = 2110 torr. In comparison with Fig. 2.7(a), the table value corresponding to P_H2 = 2105 is also read as P_H2 = 2110.
//Therefore the values of the constants are
```

```
different from that obtained in the textbook.
Also regression is used to obtain the values of
slopes and intercept whereas the textbook
considers graphical method for the computation of
 the codes
```

# Chapter 3

# Ideal Reactors

**Scilab code Exa 3.1** Time to reach desired conversion for bimolecular batch reactio

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc.,USA,pp 436.
//Chapter-1 Ex3.1 Pg No.84
//Title:Time to reach desired conversion for bimolecular batch reaction
//
clear
clc
//INPUT
C_A0=1;//Assuming 1mol basis for the limiting reactant
C_B0_old=1.02;//2% Excess of reactant B is supplied
R_old=C_B0_old/C_A0;//Refer equation 3.7 Pg No.
X_A=0.995;// Conversion interms of limiting reactant
t_old=6.5;//Time required for the given conversion (hr)
C_B0_new=1.05;//5% Excess of reactant B
```

```
R_new=C_B0_new/C_A0;//Refer equation 3.7 Pg No.83

//CALCULATION
k=(log((R_old-X_A)/(R_old*(1-X_A)))/((R_old-1)*t_old*C_A0));
t_new=log((R_new-X_A)/(R_new*(1-X_A)))/((R_new-1)*k*C_A0);

//OUTPUT
mprintf('\nTime required to achieve required conversion for 5%% excess of B= %f hr',t_new);

//FILE OUTPUT
fid=mopen('.\Chapter3-Ex1-Output.txt','w');
mfprintf(fid,'\nTime required to achieve required conversion for 5%% excess of B= %f hr',t_new);
mclose(fid);
//==================================END OF PROGRAM==================================
```

**Scilab code Exa 3.2** Residence time and heat generation for four STR s in series

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc.,USA,pp 436.
//Chapter-3 Ex3.2 Pg No. 96
//Title:Residence time and heat generation for four STR's in series
//==============================================================================

clear
clc
// COMMON INPUT
```

```
X_A=0.95;//Given conversion
t_batch=6;//Batch time to reach the desired conversion
N=4//No.of reactors in series
X_final=X_A;

//CALCULATION (Ex3.2.a)
k=log((1/(1-X_A)))/t_batch;//Refer equation 3.29 Pg No. 90
t_1=((1/(1-X_A))^(1/N)-1)/k;//Refer equation 3.40 Pg No. 94
t_Tot=N*t_1;

//OUTPUT (Ex3.2.a)
mprintf('\n OUTPUT Ex3.2.a');
mprintf('\n ==========================================================================================
');
mprintf('\nThe total residence time of the four reactors in series= %f hr',t_Tot);

//==========================================================================================

//Title:Heat generation in CSTR in Series
//==========================================================================================
//CALCULATION (Ex3.2.b)
t_1=((1/(1-X_final))^(1/N)-1)/k;//Refer equation 3.40 Pg No. 94
for i=1:N
    X(i)=1-(1/(1+k*t_1)^(i));
end

delQ_by_Q(1)=(X(1))/X_final; //  Ratio of heat generated in 1st reactor
```

```
for i=1:N-1
    delQ_by_Q(i+1)=(X(i+1)-X(i))/X_final;  // Ratio of heat generated in 2nd, 3rd and 4th reactors
end

//OUTPUT (Ex3.2.b)
mprintf('\n
=================================================================
n')
mprintf('\n OUTPUT Ex3.2.b');
mprintf('\n
=================================================================
');
mprintf('\nReactor vessel \t Conversion \t Fraction of total heat released \n')
mprintf('\n
=================================================================
')
for i=1:N
    mprintf('\n %d \t \t %0.3f \t \t \t %0.3f \n',i,X(i),delQ_by_Q(i))
end

//FILE OUTPUT
fid=mopen('.\Chapter3-Ex2-Output.txt','w');
mfprintf(fid,'\n OUTPUT Ex3.2.a');
mfprintf(fid,'\n
=================================================================
');
mfprintf(fid,'\nThe total residence time of the four reactors in series= %f hr',t_Tot);
    mfprintf(fid,'\n
    =============================================================
    ')
    mfprintf(fid,'\nReactor vessel \t Conversion \t Fraction of total heat released \n')
    mfprintf(fid,'\n
==========================================================')
for i=1:N
    mfprintf(fid,'\n %d \t \t %0.3f \t \t \t %0.3f \n',i,X(i),delQ_by_Q(i))
end
mclose(fid);


//==================================================================END OF PROGRAM==================================================
```

**Scilab code Exa 3.3** Effect of temperature on yield

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc.,USA,pp 436.
//Chapter-3 Ex3.3 Pg No. 97
//Title:Effect of temperature on yield
//==================================================================

clear
clc
//INPUT
C_A0=1;//Initial concentration of A
C_B0=5;//Initial concentration of B
E1=15;//Activation energy for first reaction(kcal)
E2=20;//Activation energy for second reaction(kcal)
X_A=0.88;// Total conversion of reactant A
Y=0.81;//Yield for the reaction to produce C
R=1.987;//Gas Constant(cal/K^-1 mol^-1)
T_0=350;//Temperature (K)
```

```

//CALCULATION
//Assuming first order by taking concentration of B constant since B is in Excess
C_A= C_A0*(1-X_A);//Unreacted amount of A
C_B=C_B0-Y;//Unreacted amount of B
k1_plus_k2_t=(X_A/(1-X_A));
S=Y/X_A;//At 350K
k1_by_k2=11.57;
k1_plus_k2_by_k2=k1_by_k2+1;//Refer Ex3.3 for the coded equations
k2_t=k1_plus_k2_t/k1_plus_k2_by_k2;
k1_t=k1_plus_k2_t-k2_t;
T=345;
for i=1:7
T=T+5;
Temp(i)=T;
k1_dash_t(i)=k1_t*exp(((E1*1000/R)*((1/T_0)-(1/T))));//Arrhenius law
k2_dash_t(i)=k2_t*exp(((E2*1000/R)*((1/T_0)-(1/T))));//Arrhenius law
k1_plus_k2_t_new(i)=k1_dash_t(i)+k2_dash_t(i);
X_A_new(i)=k1_plus_k2_t_new(i)/(1+k1_plus_k2_t_new(i));
S_new(i)=((k1_dash_t(i)/k2_dash_t(i))/(1+(k1_dash_t(i)/k2_dash_t(i))));
Y_new(i)=S_new(i)*X_A_new(i);
end

//OUTPUT
mprintf('==============================================');
mprintf('\n\t T \t X_A \t S \t Y');
mprintf('\n\t K \t (-) \t (-) \t (-)');
mprintf('\n==============================================');
for i=1:7
    mprintf('\n\t %d \t %0.3f \t %0.3f \t %0.3f',Temp(i),X_A_new(i),S_new(i),Y_new(i));
end
```

```
  maximum=max(Y_new);
  mprintf('\n\t\nThe maximum value of yield is %f ',maximum);
  mprintf('\n\t\nHigh yield is obtained between 365K to 375K');

//FILE OUTPUT
fid=mopen('.\Chapter3-Ex3-Output.txt','w');
mfprintf(fid,'==================================================');
mfprintf(fid,'\n\t T \t  X_A \t  S \t  Y');
mfprintf(fid,'\n\t K \t (-) \t  (-) \t (-)');
mfprintf(fid,'\n================================================');
for i=1:7
    mfprintf(fid,'\n\t %d \t %0.3f \t %0.3f \t %0.3f',Temp(i),X_A_new(i),S_new(i),Y_new(i));
end
  maximum=max(Y_new);
  mfprintf(fid,'\n\t\nThe maximum value of yield is %f ',maximum);
  mfprintf(fid,'\n\t\nHigh yield is obtained between 365K to 375K');
  mclose(fid);
//===================================================================
  END OF PROGRAM
  ================================================================

//Disclaimer:Refer Ex3.3 in the textbook The Arrhenius law equation has a typo error. Exponential term missing in the textbook
```

**Scilab code Exa 3.4** Volume of reactor for Gas Phase isothermal reaction

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition ) Marcel Dekker,Inc.,USA,pp 436.
//Chapter-3 Ex3.4 Pg No. 101
//Title:Volume of reactor for Gas Phase isothermal reaction
//

clear
clc
//INPUT
//First Order Reaction
//Basis: 1mol of feed
k=0.45;//Rate constant of first order reaction(s-1)
v0=120;//Volumetric flow rate(cm3/s)
C_A0=0.8;//Initial amount of reactant A (mol)
X_A=0.95;//Conversion in terms of reactant A
C_inert=0.2;//Concentration of inert (Nitrogen)in feed

//CALCULATION
E_A=((2*C_A0+C_inert)-(C_A0+C_inert))/(C_A0+C_inert);//Volume fraction
Tot_mol=(C_A0+C_inert)+(E_A);//Total No. of moles
V=v0*((-(E_A)*X_A)+Tot_mol*(log(1/(1-X_A))))/(k);//Refer Performance Equation equation 3.44 and 3.42 in Pg No. 100
V_l=V*10^-3;//Volume of reactor in liters

//OUTPUT
mprintf('\n\tThe Volume of the reactor required for the given conversion is %.0f cm3 or %0.2f liters',V,V_l);

//FILE OUTPUT
fid= mopen('.\Chapter3-Ex4-Output.txt','w');
```

```
mfprintf(fid,'\n\tThe Volume of the reactor required for the given conversion is %.0f cm3 or %0.2f liters',V,V_l);
mclose(fid);
//==================================================================END OF PROGRAM==============================================
```

**Scilab code Exa 3.5** Rate Equation to fit Initial Rate data

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc.,USA,pp 436.
//Chapter-3 Ex3.5 Pg No. 104
//Title: Rate Equation to fit Initial Rate data
//==========================================================================================================================

clear
clc
clf()
function [coefs]=regress(x,y)
coefs=[]
  if (type(x) <> 1)|(type(y)<>1) then error(msprintf(gettext("%s: Wrong type for input arguments: Numerical expected.\n"),"regress")), end
  lx=length(x)
  if lx<>length(y) then error(msprintf(gettext("%s: Wrong size for both input arguments: same size expected.\n"),"regress")), end
  if lx==0 then error(msprintf(gettext("%s: Wrong
    size for input argument #%d: Must be > %d.\n"), "regress", 1, 0)), end
  x=matrix(x,lx,1)
  y=matrix(y,lx,1)
  xbar=sum(x)/lx
  ybar=sum(y)/lx
  coefs(2)=sum((x-xbar).*(y-ybar))/sum((x-xbar).^2)
  coefs(1)=ybar-coefs(2)*xbar
endfunction
//INPUT (Ex3.5.1)
//Initial Rate Data
B_by_A= [5 7 10 20 37];//B/A Mol Ratio
r_0=[75 65 50 33 18];//Rate (mol/hr g)

//CALCULATION (Ex3.5.1)
//Assuming Eley Rideal Mechanism for the benzene alkylation with propylene
for i=1:5
    C_B(i)= (B_by_A(i)/(1+B_by_A(i)));//In terms of Mol Fraaction
    C_A(i)= (1/(1+B_by_A(i)));
    CA_CB(i)=C_B(i)*C_A(i);
    C_by_r(i)=CA_CB(i)/r_0(i);
end
coefs=regress(C_A,C_by_r);//The equation ((C_B*C_A)/r_0)= 1/(k*K_A) + (C_A/k)
scf(0)
plot(C_A,C_by_r,'*');
xtitle('Test of Eley-Rideal model for benzene alkylation');
xlabel(' CA ,Mol Fraction');
ylabel('CA CB/r_0');
intercept=coefs(1);
slope=coefs(2);
K_A=slope/intercept;
k=1/(slope);
K_A_k=k*K_A;

```

```
//OUTPUT (Ex3.5.1)
mprintf('\n OUTPUT Ex3.5.1');
mprintf('\n ========================================================================')
mprintf('\nThe rate equation for Eley-Ridely Mechanism is:\n      r= %0.0fC_A C_B/(1+%0.2fC_A)',K_A_k,K_A);
//=============================================================================================

//Title:Conversion as a function of Space velocity
//=============================================================================================
//INPUT (Ex3.5.2)
x= [0.16 0.31 0.40 0.75];
Exp_Inverse_WHSV=(10^-3)*[4 8.2 17 39];//Weight Hourly Space Velocity
Feed_ratio=10;

//CALCULATION (Ex3.5.2)
//The integrated rate equation in terms of conversion ln(1/(1-X))+0.236X= 60.4/WHSV (Page no. 106)
function [y]=integrated_rate_eqn(x0)
    y=log(1 ./(1-x0))+ 0.236.*x0 - 60.4.*Exp_Inverse_WHSV
endfunction

n=length(x)
x0=0.9*ones(1,n);  // Provide guess value for conversion
[x_predicted]=fsolve(x0,integrated_rate_eqn,1d-15); // Using fsolve to determine conversion from integrated rate expression for each operating WHSV
```

```

scf(1)
plot(Exp_Inverse_WHSV,x,'*',Exp_Inverse_WHSV,x_predicted,'--')
xtitle('Integral analysis','Inverse of WHSV','Conversion')
legend('Experimental','Predicted')

//OUTPUT (Ex3.5.2)
//Console Output
mprintf('\n==============================================================\n');
mprintf('\n OUTPUT Ex3.5.2');
mprintf('\n Predicted and Experimental Conversion Values')
mprintf('\n==============================================================')
mprintf('\n10^3/WHSV\tX_experimental\tX_predicted')
mprintf('\n==============================================================')
for i=1:n
    mprintf('\n %0.2f\t\t%0.2f\t\t%0.2f  ',Exp_Inverse_WHSV(i)*10^3,x(i),x_predicted(i))
end

//FILE OUTPUT
fid= mopen('.\Chapter3-Ex5-Output.txt','w');
mfprintf(fid,'\n OUTPUT Ex3.5.1');
mprintf('\n==============================================================')
mfprintf(fid,'\nThe rate equation for Eley-Ridely Mechanism is:\n      r= %0.0fC_A C_B/(1+%0.2fC_A)',K_A_k,K_A);
mfprintf(fid,'\n
==========================================================\n')
mfprintf(fid,'\n OUTPUT Ex3.5.2');
mfprintf(fid,'\n Predicted and Experimental Conversion Values')
mfprintf(fid,'\n ==========================================================')
mfprintf(fid,'\n10^3/WHSV\tX_experimental\tX_predicted')
mfprintf(fid,'\n ==========================================================')
for i=1:n
  mfprintf(fid,'\n %0.2f\t\t%0.2f\t\t%0.2f  ',Exp_Inverse_WHSV(i)*10^3,x(i),x_predicted(i))
end
mclose(fid)

//====================================================END OF PROGRAM======================================
//Disclaimer:Regression method is used to find the slope and intercept in Ex3.5.2 .
// Hence the rate equation differ from the graphically obtained values of slope and intercept in the textbook.
```

**Scilab code Exa 3.6** Optimum reaction temperature

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc.,USA,pp 436.
//Chapter-3 Ex3.6 Pg No. 114
//Title: Optimum reaction temperature
```

```
//==========================================================
clear
clc
//INPUT
del_H=-20*10^3;//Heat of reaction(cal)
T_eq=[500 700];//Equivalent temperatures (K)
R=1.987;//Gas Constant (cal/mol K)
E2_by_E1=2;//Ratio of activation energy

//CALCULATION
T_opt(1)=T_eq(1)/(1+(log(E2_by_E1)*(R/(-del_H)))*T_eq(1));//Refer equation 3.63 Pg No. 113
T_opt(2)=T_eq(2)/(1+(log(E2_by_E1)*(R/(-del_H)))*T_eq(2));
delta_T(1)=T_eq(1)-T_opt(1);
delta_T(2)=T_eq(2)-T_opt(2);


//OUTPUT
mprintf('\n  \t   \t Temperature_1\t Temperature_2  ');
mprintf('\n  \t   \t ==========================================');
mprintf('\n(T_eq - T_opt)(K):  \t%0.0f      \t\t%0.0f  ',delta_T(1),delta_T(2));
mprintf('\n   T_opt(K):\t \t%0.0f\t\t%0.0f', T_opt(1),T_opt(2));

fid= mopen('.\Chapter3-Ex6-Output.txt','w');
mfprintf(fid,'\n  \t   \t Temperature_1\t Temperature_2  ');
mfprintf(fid,'\n  \t   \t ==========================================');
mfprintf(fid,'\n(T_eq - T_opt)(K):  \t%0.0f      \t\t%0.0f',delta_T(1),delta_T(2));
mfprintf(fid,'\n   T_opt(K):\t \t%0.0f\t\t%0.0f',
T_opt(1),T_opt(2));
mclose(fid);

//================================================================
END OF PROGRAM==================================================
//Disclaimer:There is an arithmetic error in  the optimum temperatures obtained in the textbook.
// Based on the values (T_eq - T_opt)1=17 and  (T_eq - T_opt)2=32 the optimum temperatures obtained are
// T_opt1=483 K and T_opt2=668 K respectively.
```

**Scilab code Exa 3.7** Equilibrium temperature as a function of conversion and optimu

```
//Harriot P,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc. USA,pp 436
//Chapter-3 Ex3.7 Pg No. 115
//Title:Equilibrium temperature as a function of conversion and Optimum Feed Temperature
//================================================================

clear
clc
// COMMON INPUT
P_opt=1.5; //(atm) Operating pressure of first converter
x=[0.5 0.6 0.7 0.8 0.9 0.95];// Conversion of SO2
k=[2E-06 5.1E-06 10.3E-06 18E-06 27E-06 37.5E-06 48E
```

```
   -06 59E-06 69E-06 77E-06] ; //Rate Constant (gmol
   /g cat sec atm)
T=420:20:600;// Temperature ( C )
X=0.68;
T_F=700;//Feed Temperature(K)
C_pi_800=[12.53 18.61 8.06 7.51];
F=100;// (mol) amount of feed
delta_H_700=-23270;//(cal/mol)
percent_SO2_f=11;//(%)Percentage of SO2 in feed


//CALCULATION (Ex3.7.a)
n=length(x);
m=length(k);
for i=1:n
    K_eq(i)=((x(i)/(1-x(i))))*((100-5.5*x(i))
       /(10-5.5*x(i)))^0.5*(1/P_opt)^0.5;
    T_eq(i)=(11412/(log(K_eq(i))+10.771));
    P_O2(i)=(10*(10-5.5*x(i))*P_opt)/(100-5.5*x(i));
    P_SO3(i)=(11*x(i)*P_opt)/(100-5.5*x(i));
    P_SO2(i)=(11*(1-x(i))*P_opt)/(100-5.5*x(i));
end

for i=1:n
    for j=1:m
        r(j,i)=k(j)*(P_SO2(i)/P_SO3(i))^0.5*(P_O2(i)
           -(P_SO3(i)/(P_SO2(i)*K_eq(i)))^2)
    end
    r_max(i)=max(r(j,i));
end
clf()
scf(0)
plot(x,T_eq-273,'*');
xtitle('Temperature in Stage 1 of an SO2 converter')
   ;
xlabel('x,SO2 Conversion');
ylabel('Temperature, C ' );

```

```
//CALCULATION (Ex3.7.b)
n_SO2=F*percent_SO2_f*10^-2*(1-X);
n_SO3=F*percent_SO2_f*10^-2*X;
n_O2=(10-5.5*X);
n_N2=79;
sigma_n_C_pi=n_SO2*C_pi_800(1)+n_SO3*C_pi_800(2)+n_O2*C_pi_800(3)+n_N2*C_pi_800(4);
Temp_change=(F*percent_SO2_f*10^(-2)*X*(-1)*delta_H_700)/sigma_n_C_pi;//Refer equation 3.60 Pg No.110
mprintf('\nHeat Capacity evaluated at 800 K :%0.0f (cal/ C )',sigma_n_C_pi);
mprintf('\nTemperature Change to carry out the reaction at T_F,\nusing the energy to heat the product gas :%0.0f  C ",Temp_change);
//From graphical procedure (Figure 3.19 ,Pg No.118) the final temperature is obtained as 410  C
T_F=410;//( C ) Final temperature
//From Figure 3.19 ,Pg No.118 temperature for corresponding conversion is obtained
X_stage=[0.1;0.2;0.3;0.4;0.5;0.6]
T_stage=[441;470;500;540;565;580]
m=length(X_stage);
for i=1:m
    K_eq(i)=exp((11412/T_stage(i))-10.771);
end
k=10^-6*[5.25 14.15 27 48 61.5 69];//From Table 3.5 Corresponding to the stage temperature data obtained form Figure 3.19
for i=1:m
    P_SO2(i)=11*(1-X_stage(i))*P_opt/(100-5.5*X_stage(i))
    P_SO3(i)=11*X_stage(i)*P_opt/(100-5.5*X_stage(i))
    P_O2(i)=10*(10-5.5*X_stage(i))*P_opt/(100-5.5*X_stage(i))
    r(i)=k(i)*(P_SO2(i)/P_SO3(i))^0.5*(P_O2(i)-(P_SO3(i)/(P_SO2(i)*K_eq(i)))^2)*10^6;
    inverse_r(i)=(1/r(i));
end
scf(1)
 plot(X_stage,inverse_r,'*');
 xtitle('1/r vs x','X (conversion)','10^-6/r');


//OUTPUT (Ex3.7.a)
mprintf('\n\n OUTPUT Ex3.7.a');
mprintf('\n ================================================================================');
mprintf('\n X\tPhi\t\tT_eq\tT_eq\t\tr_max');
mprintf('\n -\t(atm^-0.5)\t(K)\t( C )\t\t(gmol/g cat sec)');
mprintf('\n ================================================================================');
for i=1:n-1
    mprintf('\n %0.2f\t%0.2f\t %0.0f\t%0.0f\t\t%0.6E',x(i),K_eq(i),T_eq(i),T_eq(i)-273,r_max(i));
end
mprintf('\n %0.2f\t%0.2f\t\t%0.0f\t%0.0f\t\t%0.6E',x(n),K_eq(n),T_eq(n),T_eq(n)-273,r_max(n));

//OUTPUT (Ex3.7.b)
mprintf('\n\n\n OUTPUT Ex3.7.b');
mprintf('\n ================================================================================');
 mprintf('\n ==============================================');
 mprintf('\n 10^-6/r\tX (conversion)');
 mprintf('\n (gmol/g cat,s) \t(-)');
 mprintf('\n ==============================================');
 for i=1:m
    mprintf('\n %0.2f\t\t\t%0.2f',inverse_r(i),
        X_stage(i));
 end
 mprintf('\nFrom graphical procedure (1/r vs x) the optimum temperature obtained is T_opt: 412 C ');

// FILE OUTPUT
fid= mopen('.\Chapter3-Ex7-Output.txt','w');
mfprintf(fid,'\nHeat Capacity evaluated at 800 K :%0.0f (cal/ C )',sigma_n_C_pi);
mfprintf(fid,'\nTemperature Change to carry out the reaction at T_F,\nusing the energy to heat the product gas :%0.0f  C ”,Temp_change);
mfprintf(fid,'\n OUTPUT Ex3.7.a’);
mfprintf(fid,'\n==================================================================
');
mfprintf(fid,'\n X\tPhi\t\tT_eq\tT_eq\t\tr_max');
mfprintf(fid,'\n -\t(atm^-0.5)\t(K)\t( C )\t\t(gmol/g cat sec)');
mfprintf(fid,'\n==================================================================
');
for i=1:n-1
    mfprintf(fid,'\n %0.2f\t%0.2f\t %0.0f\t%0.0f\t\t%0.6E',x(i),K_eq(i),T_eq(i),T_eq(i)-273,r_max(i));
end
mfprintf(fid,'\n %0.2f\t%0.2f\t\t%0.0f\t%0.0f\t\t%0.6E',x(n),K_eq(n),T_eq(n),T_eq(n)-273,r_max(n));
mfprintf(fid,'\n\n\n OUTPUT Ex3.7.b');
mfprintf(fid,'\n==================================================================
');
 mfprintf(fid,'\n==================================================');
 mfprintf(fid,'\n 10^-6/r\tX (conversion)');
 mfprintf(fid,'\n (gmol/g cat,s) \t(-)');
 mfprintf(fid,'\n
==================================================');
for i=1:m
    mfprintf(fid,'\n %0.2f\t\t\t%0.2f',inverse_r(i),X_stage(i));
end
mfprintf(fid,'\nFrom graphical procedure (1/r vs x) the optimum temperature obtained is T_opt: 412 C ');
mclose(fid);

//====================================================================END OF PROGRAM==============================================
//Disclaimer: The optimum temperature for each conversion is found by trial at maximum rate and the kinetic data in the textbook is not sufficient to calculate the optimum temperature in the code.
```

# Chapter 4

# Diffusion and Reaction in Porous Catalysts

**Scilab code Exa 4.1** Diffusivity of Chlorine and tortuosity in catalyst pellet

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc.,USA,pp 436.
//Chapter-4 Ex4.1 Pg No. 135
//Title:Diffusivity of Chlorine and tortuosity in catalyst pellet
//==================================================================================

clear
clc

// COMMON INPUT
S_g=235;//Total surface per gram (m2/g)
V_g=0.29E-6;//Pore volume per gram (cm3/g)
rho_p=1.41;//Density of particle (g/cm3)
D_He=0.0065;//Effective diffusivity of He (cm2/sec)
D_AB=0.73;// at 1atm and 298K
```

```
M_He=4;//Molecular weight of He
M_Cl2=70.09;//Molecular weight of Cl2
T_ref=293;//Reference temperature
T_degC=300;
T_01=T_degC+273;//Reaction temperature(K) (Ex4.1.a)
T_02=298;//Operating temperature  (Ex4.1.b)
T_03=573;//operating temperature (Ex4.1.c)
P_ref=1;//Reference pressure
D_Cl2_CH4=0.15;//at 1atm 273K
P=15;//operating pressure
//tau=1.25;//From value calculated in Ex4.1.b Pg. No. 136


//CALCULATION (Ex4.1.a)
r_bar=2*V_g/S_g;//Mean Pore radius
D_Cl2_Ex_a=D_He*((M_He/M_Cl2)*(T_01/T_ref))^(0.5);//Assuming Knudsen flow at 573K

//CALCULATION (Ex4.1.b)
r_bar=2*V_g*(10^6)/(S_g *(10^4));
D_K=9700*(r_bar)*(T_ref/M_He)^(0.5);//Knudsen flow
D_AB1=D_AB*(293/298)^(1.7)// at 1.5 atm and 293K
D_pore=1/((1/D_K)+(1/D_AB1));//pore diffusion
Epsilon=V_g*rho_p*(10^6);
tau=(D_pore*Epsilon)/D_He;//Tortusity

//CALCULATION (Ex4.1.c)
D_Cl2_CH4_new=D_Cl2_CH4*(P_ref/P)*(T_03/T_ref)^(1.7);
D_K_Cl2=9700*r_bar*sqrt(T_03/M_Cl2);
D_pore=1/((1/D_Cl2_CH4_new)+(1/D_K_Cl2));
Epsilon=V_g*rho_p;
D_Cl2_Ex_c=D_pore*Epsilon/tau;


//OUTPUT
mprintf('\n OUTPUT Ex4.1.a');
mprintf('\n==============================================================');
mprintf('\nThe predicted diffusivity of Chlorine is %0.2e cm2/s ',D_Cl2_Ex_a);
mprintf('\n\n OUTPUT Ex4.1.b');
mprintf('\n==============================================================');
mprintf('\nThe tortusity value = %0.2f',tau);
mprintf('\n\n OUTPUT Ex4.1.b');
mprintf('\n==============================================================')
mprintf('\nThe Effective diffusivity of Chlorine at %g K and %g atm =  %0.2e cm2/sec ',T_03, P, D_Cl2_Ex_c);

//FILE OUTPUT
fid= mopen('.\Chapter4-Ex1-Output.txt','w');
mfprintf(fid,'\n OUTPUT Ex4.1.a');
mfprintf(fid,'\n==============================================================');
mfprintf(fid,'\nThe predicted diffusivity of Chlorine is %0.2e cm2/s ',D_Cl2_Ex_a);
mfprintf(fid,'\n\n OUTPUT Ex4.1.b');
mfprintf(fid,'\n==============================================================');
mfprintf(fid,'\nThe tortusity value = %0.2f',tau);
mfprintf(fid,'\n\n OUTPUT Ex4.1.b');
mfprintf(fid,'\n==============================================================')
mfprintf(fid,'\nThe Effective diffusivity of Chlorine at %g K and %g atm =  %0.2e cm2/sec ',T_03, P, D_Cl2_Ex_c);
```

```
mclose(fid)
//====================================================END OF PROGRAM============================================================
```

**Scilab code Exa 4.2** Effective diffusivity of O2 in air

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc.,USA,pp 436.
//Chapter-4 Ex4.2 Pg No. 140
//Title:Effective diffusivity of O2 in air
//================================================================================================

clear
clc
// COMMON INPUT
S_g=150;//Total surface per gram (m2/g)
V_g=0.45;//Pore volume per gram (cm3/g)
V_i=0.30;//Micropore volume per gram (cm3/g)
V_a=0.15;// Macropore volume per gram (cm3/g)
rho_P=1.2;//Density of particle (g/cm3)
tau=2.5;// Tortusity
r_bar_i=40*(10^(-8));//Micropore radius
r_bar_a=2000*(10^(-8));//Macropore radius
D_AB=0.49;//For  N2 O2  at 1 atm (cm2/s)
M_O2=32;//Molecular weight of O2
T=493;//Opereating Temperature (K)



//CALCULATION (Ex4.2.a)
Epsilon=V_g*rho_P;
```

```
D_K_i=9700*(r_bar_i)*sqrt(T/M_O2);//Knudsen flow for micropore
D_Pore_i=1/((1/D_K_i)+(1/D_AB))
D_K_a=9700*(r_bar_a)*sqrt(T/M_O2);
D_Pore_a=1/((1/D_K_a)+(1/D_AB));////Knudsen flow for macropore
D_Pore_Avg=(V_i*D_Pore_i+V_a*D_Pore_a)/(V_i+V_a);
D_e=Epsilon*D_Pore_Avg/tau;

//CALCULATION (Ex4.2.b)
Epsilon=V_g*rho_P;
r_bar=2*V_g/(S_g*10^4);
D_K=9700*(r_bar)*sqrt(T/M_O2);//Knudsen Flow
D_Pore=1/((1/D_K)+(1/D_AB));
tau=D_Pore*Epsilon/D_e;

//OUTPUT
mprintf('\n OUTPUT Ex4.2.a');
mprintf('\n ==========================================================================================');
mprintf('\n The effective diffusivity of O2 in air = %0.2e cm2/s',D_e);
mprintf('\n\n OUTPUT Ex4.2.b');
mprintf('\n ==========================================================================================');
mprintf('\n The calculated surface mean pore radius = %.0e cm',r_bar);
mprintf('\n The predicted pore diffusivity = %0.2e cm2/sec',D_Pore);
mprintf('\n The corresponding tortusity = %0.2f',tau);

//FILE OUTPUT
fid= mopen('.\Chapter4-Ex2-Output.txt','w');
mfprintf(fid,'\n OUTPUT Ex4.2.a');
mfprintf(fid,'\n
==================================================
');
mfprintf(fid,'\n The effective diffusivity of O2 in air = %0.2e cm2/s',D_e);
mfprintf(fid,'\n\n OUTPUT Ex4.2.b');
mfprintf(fid,'\n ==================================================');
mfprintf(fid,'\n The calculated surface mean pore radius = %.0e cm',r_bar);
mfprintf(fid,'\n The predicted pore diffusivity = %0.2e cm2/sec',D_Pore);
mfprintf(fid,'\n The corresponding tortusity = %0.2f',tau);
mclose(fid);


//=======================================================END OF PROGRAM========================================
```

**Scilab code Exa 4.3** Influence of Pore diffusion over rate

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc.,USA,pp 436.
//Chapter-4 Ex4.3 Pg No. 154
//Title:Influence of Pore diffusion over rate
//=================================================================
clear
clc
```

```
//INPUT
d_p=1/4;//Spherical Catalyst pellet size(inch)
k=[7.6*10^-3 14*10^-3];//Reaction rates (mol/hr)
f_A=[0.1 0.2];//Feed fraction of reactant A
D_e=0.0085;// Diffusivity of A (cm2/s)
rho_p=1.4 ;// Density of catalyst particle(g/cm3)
V_ref=22400;// reference volume(cm3)
T_ref=273;//Reference Temperature (K)
P_ref=1;//Reference Pressure (atm)
P=1.2;//Operating Pressure (atm)
T_C=150;
T=T_C+273;//Operating Temperature (K)

//CALCULATION
//For 10% of A
C_A(1)=f_A(1)*T_ref*P_ref/(V_ref*T*P);
R=d_p*2.54/2;
k_app(1)=k(1)*rho_p/(3600*C_A(1));//Refer equation 4.53 Pg. No. 153
phi_app(1)=R*sqrt(k_app(1)/D_e);//Refer equation 4.55 Pg. No. 155
C_A(2)=f_A(2)*T_ref*P_ref/(V_ref*T*P);
//If C_A is doubled the order is quite close to 1, from the Figure 4.8 Pg. No. 148, refer value of effectiveness
eta_graph=0.42;
k_app(2)=k_app(1)/eta_graph;
phi_app(2)=R*sqrt(k_app(2)/D_e);
eta_calc=(3/phi_app(2))*((1/tanh(phi_app(2)))-(1/phi_app(2)));
eff_rate=(1-eta_graph)*100;

//OUTPUT
mprintf('\n The effectiveness from graph = %0.2f \n The calculated effectiveness = %0.2f',eta_graph,eta_calc);
mprintf('\n The pore diffusion decreased the rate by %.0f%%',eff_rate);
```

```

//FILE OUTPUT
fid= mopen('.\Chapter4-Ex3-Output.txt','w');
mfprintf(fid,'\n The effectiveness from graph = %0.2f \n The calculated effectiveness = %0.2f',eta_graph,eta_calc);
mfprintf(fid,'\n The pore diffusion decreased the rate by %.0f%%',eff_rate);
mclose(fid);
//==============================================================================END OF PROGRAM========================================
```

**Scilab code Exa 4.4** Effectiveness factor for solid catalyzed reaction

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc. USA,pp 436.
//Chapter-4 Ex4.4 Pg No.157
//Title: Effectiveness factor for solid catalyzed reaction
//==================================================================================

clear
clc
//INPUT
D_e_A=0.02;//(cm2/s)
D_e_B=0.03;//(cm2/s)
D_e_C=0.015;//(cm2/s)
X_f_A=0.3;
X_f_B=(1-X_f_A);
eta_assumed=0.68;//Effectiveness factor from Fig.4.8 for first order reaction
```

```
T=150;//(deg C)
T_K=T+273;//(K)
r=0.3;//(cm)Radius of catalyst sphere
P_opt=4;//(atm)Operating Pressure
R=82.056;//(cm3 atm/K mol)Gas constant


//CALCULATION
//Kinetic equation r= (2.5*10^-5*P_A*P_B)/(1+0.1*P_A+2*P_C)^2
P_A=X_f_A*P_opt;
P_B=X_f_B*P_opt;
r_star=(2.5*10^-5*P_A*P_B)/(1+0.1*P_A)^2;
C_A=P_A/(R*T_K);
k=r_star/C_A;
Phi= r*(k/D_e_A)^(0.5);
P_A_bar=eta_assumed*P_A;
delta_P_A=P_A*(1-eta_assumed);
delta_P_B=delta_P_A*(D_e_A/D_e_B);
P_B_bar=P_B-delta_P_B;
delta_P_C=delta_P_A*(D_e_A/D_e_C);
P_C_bar=delta_P_C;
r_calc=(2.5*10^-5*P_A_bar*P_B_bar)/(1+0.1*P_A_bar+2*P_C_bar)^2
eta_calc=r_calc/r_star;
eta_approx=(eta_calc+eta_assumed)/2;

//OUTPUT
//Console Output
mprintf('\tBased on average pressures calculated Rate and Effectiveness factor');
mprintf('\n\t r : %0.2E (mol/s cm3)',r_calc);
mprintf('\n\t eta_calc : %0.3f ',eta_calc);
mprintf('\n The actual value of Effectiveness factor eta_actual :%0.1f',eta_approx);

//File Output
fid= mopen('.\Chapter4-Ex4-Output.txt','w');
```

```
mfprintf(fid,'\tBased on average pressures calculated Rate and Effectiveness factor');
mfprintf(fid,'\n\t r : %0.2E (mol/s cm3)',r_calc);
mfprintf(fid,'\n\t eta_calc : %0.3f ',eta_calc);
mfprintf(fid,'\n The actual value of Effectiveness factor eta_actual :%0.1f',eta_approx);
mclose(fid);
//==================================== END OF PROGRAM ======================================================
```

**Scilab code Exa 4.5** The optimum pore size distribution for a spherical pellet

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc.,USA,pp 436.
//Chapter-4 Ex4.5 Pg No. 164
//Title:The optimum pore size distribution for a spherical pellet
//======================================================================================

clear
clc
//INPUT
d_pellet=5*10^-1;//Catalyst pellet size (cm)
k_cat =3.6;// True Rate Constant (sec-1)
V_g_cat=0.60 ;// Pore Volume of the catalyst(cm3/g)
S_g_cat=300*10^4;//Surface area of catalyst (cm2/g)
dp=0.02;// Size of powdered catalyst(cm)
rho_p=0.8 ;// Density of  catalyst particle(g/cm3)
r_bar_narrow= 40*10^(-10)//narrow distribution
D_KA=0.012 ;//(cm2/sec)
```

```
D_AB= 0.40 ;//(cm2/sec)
r_macro=2000*10^(-10);//For Macropores
V_cat=1/rho_p;//Total catalyst volume (cm3/g)
eta=1;//For powdered catalyst

//CALCULATION
epsilon=V_g_cat/V_cat;
r_bar=2*V_g_cat/S_g_cat;
R=dp/2;
R_pellet=d_pellet/2;
D_pore_a=1/((1/D_KA)+(1/D_AB));
tau=3;//Assumed value
D_e_cat=D_pore_a*epsilon/tau;
Phi_app=R*sqrt(k_cat/D_e_cat);//Refer equation 4.55 Pg. No. 153
D_KB=D_KA*(r_macro/r_bar_narrow);
D_pore_b=1/((1/D_KB)+(1/D_AB));
V_a_end=0.35;
del_V_a=-0.05;
V_a=V_g_cat:del_V_a:V_a_end;
 for i=1:6
     V_b(i)=V_g_cat-V_a(i);//Refer Equation 4.81 Pg. No. 164
     S_a(i)=2*(V_a(i)/r_bar_narrow)*(10^-6);
     S_b(i)=2*(V_b(i)/r_macro)*(10^-6);
     S_g(i)=S_a(i)+S_b(i);
     k(i)=k_cat*S_g(i)/(S_g_cat*10^-4);
     D_e(i)=((D_pore_a*V_a(i)+D_pore_b*V_b(i))/V_g_cat)*(epsilon/tau);
     phi(i)=R_pellet*sqrt(k(i)/D_e(i));
     eta(i)=(3/phi(i))*((1/tanh(phi(i)))-(1/phi(i)));
     eta_k(i)=eta(i)*k(i)
   end
 //OUTPUT
 mprintf('\n
   ==============================================================================
   ')
 mprintf('\nV_a \t V_b \t\t S_a    \t S_b \t    S_g   \t k \t D_e \t         phi\teta\teta_k');
 mprintf('\nVolume \t cm3/g \t\t Surface Area \t m2/g \t\t s-1 \t cm2/s \t         (-)\t(-) \t (-)');
  mprintf('\n====================================================================================================================================')
 for i=1:6
         mprintf('\n %.2f \t %0.2f \t\t %.0f \t %.1f \t %0.1f \t\t %0.2f \t%0.2e\t%0.2f \t %0.2f \t %0.2f',V_a(i),V_b(i),S_a(i),S_b(i),S_g(i),k(i),D_e(i),phi(i),eta(i),eta_k(i));
 end

//FILE OUTPUT
fid= mopen('.\Chapter4-Ex5-Output.txt','w');
 mfprintf(fid,'\n====================================================================================================================================')
 mfprintf(fid,'\nV_a \t V_b \t\t S_a    \t S_b \t    S_g   \t k \t D_e \t         phi\teta\teta_k');
 mfprintf(fid,'\nVolume \t cm3/g \t\t Surface Area \t m2/g \t\t s-1 \t cm2/s \t         (-)\t(-) \t (-)');
  mfprintf(fid,'\n====================================================================================================================================')
 for i=1:6
         mfprintf(fid,'\n %.2f \t %0.2f \t\t %.0f \t %.1f \t %0.1f \t\t %0.2f \t%0.2e\t%0.2f \t %0.2f \t %0.2f',V_a(i),V_b(i),S_a(i),S_b(i),S_g(i),k(i),D_e(i),phi(i),eta(i),eta_k(i));
 end
//==================================================================================================================================== END OF PROGRAM
```

# Chapter 5

# Heat and Mass Transfer in Reactors

**Scilab code Exa 5.1** Temperature Profiles for tubular reactor

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc. USA,pp 436
//Chapter-5 Ex5.1 Pg No. 185
//Title: Temperature Profiles for tubular reactor
//=================================================================
clear
clc
clf
//INPUT
delta_H=-25000;//(kcal/mol) Enthalpy
D=2;//(cm)Diameter of Tubular Reactor
C_A0=0.002;//(mol/cm3) Initial concentration of feed
k=0.00142;//(s-1) Rate Constant
```

```
E_by_R=15000;//(K−1)
rho=0.8;//(g/cm3)
c_p= 0.5;// (cal/g C)
U=0.025;//(cal/sec cm2 C )
u=60;//(cm/s)


//CALCULATION
function diffeqn = Simul_diff_eqn(l,y,T_j)
    diffeqn(1) =(k*exp(E_by_R*((1/T_initial)-(1/y(2)))))*(1-y(1))/u;// Derivative for the first variable
    diffeqn(2) =(C_A0*(k*exp(E_by_R*((1/T_initial)-(1/y(2)))))*(1-y(1))*(-1*delta_H)-U*(4/D)*(y(2)-T_j))/(u*rho*c_p) ; // Derivative for the second variable
endfunction

// ==================================================

T_j_data = [ 348 349 350 351];
m = length(T_j_data);
n = 1;
while n <= m
T_j = T_j_data(n)
T_initial=340;// for rate constant
x0=0;
T0=344;
l0=0;
l=0:0.1E2:70E2;
y = ode([x0;T0],l0,l,list(Simul_diff_eqn,T_j));
x_data(n,:) = y(1,:);
T_data(n,:) = y(2,:);
n = n + 1;
end
// =========================================
scf(0)
plot(l,T_data(1,:),'r−',l,T_data(2,:),'b−',l,T_data
    (3,:),'k-',l,T_data(4,:),'g-')
xtitle('Temperature Profiles for a jacketed  tubular
      reactor')
xlabel("Length (cm)")
ylabel("Temperature (K)")
legend(['348';'349';'350';'351']);

scf(1)
plot(l,x_data(1,:),'r-',l,x_data(2,:),'b-',l,x_data
    (3,:),'k-',l,x_data(4,:),'g-')
xtitle('Conversion for a jacketed  tubular  reactor'
    );
xlabel("Length (cm)")
ylabel("Conversion")
legend(['348';'349';'350';'351']);

//OUTPUT
mprintf('\n The Temperature profiles for four feed
    temperatures are plotted');
mprintf('\n For T0:348 K  attains its maximum
    temperature at conversion of about 25%%-30%%');
mprintf('\n At T0:351 K the temperature increases by
     6.5 C  high senstivity that the reactor is
    nearing unstable');

//FILE OUTPUT
fid= mopen('.\Chapter5-Ex1-Output.txt','w');
mfprintf(fid,'\n The Temperature profiles for four
    feed temperatures are plotted.');
mfprintf(fid,'\n For T0:348 K  attains its maximum
    temperature at conversion of about 25%%-30%%');
mfprintf(fid,'\n At T0:351 K the temperature
    increases by 6.5 C  high senstivity that the
    reactor is nearing unstable');
mclose(fid);

//
```

```
END OF PROGRAM
```

**Scilab code Exa 5.2** Maximum internal temperature difference

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc.,USA,pp 436.
//Chapter-5 Ex5.2 Pg No. 194
//Title: Maximum internal temperature difference
//
clear
format(16)
clc
//INPUT
T_C=200;//Temperature( C )
P=1.2;//Pressure (atm)
f_ethylene=0.05;//fraction of ethylene
k_s=8*10^(-4);//Solid conductivity (cal/sec cm C)
D_e=0.02;//Diffusivity for ethylene (cm2/s)
del_H= -32.7*10^(3);//Heat of reaction (cal)
V_ref=22400;// reference volume(cm3)
T_ref=273;//Reference Temperature (K)
P_ref=1;//Reference Pressure (atm)
T_K=T_C+273;//Reaction Temperature (K)

//CALCULATION
C_s=f_ethylene*P*T_ref/(V_ref*T_K*P_ref);
Tc_minus_Ts=D_e*C_s*(-del_H)/k_s;//Refer equation 5.51 Pg No. 194

```

```
//OUTPUT
mprintf('\n\tThe maximum internal temperature difference %0.3f  C ',Tc_minus_Ts);

//FILE OUTPUT
fid= mopen('.\Chapter5-Ex2-Output.txt','w');
mfprintf(fid,'\n\tThe maximum internal temperature difference %0.3f  C ',Tc_minus_Ts);
mclose(fid);

//==================================================================END OF PROGRAM==============================================================
```

**Scilab code Exa 5.3** Overall heat transfer coefficients and radial average bed temp

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc.,USA,pp 436.
//Chapter-5 Ex5.3 Pg No. 209
//Title:Overall heat transfer coefficients and radial average bed temperature for packed bed reactor
//===================================================================================

clear
clc

// COMMON INPUT
k_s= 8*10^(-4);//(cal/sec cm C)
M_air_avg=29.24;// Average Molecular weight of air
Cp_air_mol=7.91;// cal/mol C;
```

```
Cp_air_g=Cp_air_mol/M_air_avg;//cal/g C
dp=0.4;//Size of the catalyst pellet (cm)
D=3.8;//Diameter of tube (cm)
R_pellet=D/2;//Radius
f_EO=0.7;//Fraction  of ethylene forming ethylene oxide
f_CO2_H2O=1-f_EO;//Fraction  of ethylene forming CO2 and H2O
rho_p=2.5;//Density of catalyst particle (g/cm3)
V_ref=22400;//Reference volume(cm3)
T_ref=273;// Reference Temperature (K)
P_ref=1;//Reference  Pressure (atm)
P=5;//System Pressure (atm)
T_C=230;//System Temperature ( C )
T=T_C+273;//System Temperature (K)
u_ft=[1.5 3];//Velocity (ft/s)
myu=0.026*(10^(-2));//Viscosity of air (Poise)
M_wt=[28 32 44 28];//Molecular weight
M_fraction=[0.04 0.07 0.06 0.83];
Cp=[15.3 7.4 10.7 7.4];//(cal/mol C)
k_g=9.27*10^(-5);//(cal/sec cm C)
del_H_rxn=[-29.9 -317];//(kcal/mol)
E=18*1000;//Activation Energy (cal)
R=1.987;//Gas Constant (cal/K.mol)

//CALCULATION (Ex5.3.a)
rho=M_air_avg*P*T_ref/(V_ref*P_ref*T);
u=30.533.*u_ft;//Velocity in (cm/s)
Re_p=(rho*dp/myu).*u;
Pr=Cp_air_g*myu/k_g;
ks_by_kg=k_s/k_g;
k0e_by_kg=3.5;//From figure 5.16 Pg. No. 203
kr_by_kg=2.5;//From equation 5.68 and 5.69  Pg. No. 204
for i=1:2
    ktd_by_k_air(i)=(0.1*Pr)*Re_p(i);
ke_by_kg(i)=(k0e_by_kg+kr_by_kg)+ktd_by_k_air(i);
k_e(i)=ke_by_kg(i)*k_g;
```

```
h_bed(i)=4*k_e(i)/R_pellet;
Nu_w(i)=(1.94*Pr^(0.33))*Re_p(i)^(0.5);//Refer equation 5.83 Pg. No. 208
h_w(i)=(k_g/dp)*Nu_w(i);//(cal/sec cm2 K)
h_j=100*10^(-3);//Assumed
      U(i)=1/((1/h_j)+(1/h_w(i))+(1/h_bed(i)));
end

//CALCULATION (Ex5.3.b)
minus_delH=f_EO*(-del_H_rxn(1))+f_CO2_H2O*(-del_H_rxn(2));
T_max=T+20;
del_Tc= R*(T_max)^2/E;
T_new=250 +273;
X_E=0.1;
k250_by_k230=exp((E/R)*((1/T)-(1/T_new)));
P_E=P*(1-X_E)*M_fraction(1);
P_O2=P*(1-f_EO*X_E)*M_fraction(2);
P_CO2=P*(1+f_CO2_H2O*X_E)*M_fraction(3);
r=k250_by_k230*((0.076*P_E*P_O2)/(1+2*P_E+15*P_CO2));
Q_dash=r*minus_delH*10^3/3600;
epsilon=0.4;
rho_bed=rho_p*(1-0.4);
A_percm3=4/D;
Q=(Q_dash*rho_bed)
for i=1:2
    delta_T(i)=(Q/A_percm3)*(1/U(i));
end

//OUTPUT ((Ex5.3.a))
mprintf('\n OUTPUT Ex5.3.a');
mprintf('\n ============================================================')
mprintf('\nThe Overall Heat transfer coefficient for given Velocities' )
mprintf('\n
==================================================================')
mprintf('\n  u(velocity)      U')
mprintf('\n  (ft/s)      (cal/cm2 sec K)')
mprintf('\n==================================================================')
for i=1:2
    mprintf('\n %0.1f      %3E',u_ft(i),U(i))
end

//OUTPUT ((Ex5.3.b)
mprintf('\n\n\n OUTPUT Ex5.3.b');
mprintf('\n==================================================================')
mprintf('\nThe Peak Radial average bed temperature for given Velocities' )
mprintf('\n==================================================================')
mprintf('\n  u(velocity)      delta_T')
mprintf('\n  (ft/s)             ( C )')
mprintf('\n==================================================================')
for i=1:2
    mprintf('\n  %0.1f \t  \t  %0.0f',u_ft(i),delta_T(i))
end

//FILE OUTPUT
fid= mopen('.\Chapter5-Ex3-Output.txt','w');
mfprintf(fid,'\n OUTPUT Ex5.3.a');
mfprintf(fid,'\n==================================================================')
mfprintf(fid,'\nThe Overall Heat transfer
    coefficient for given Velocities' )
mfprintf(fid,'\n
=========================================================================
    ')
mfprintf(fid,'\n  u(velocity)      U')
mfprintf(fid,'\n  (ft/s)      (cal/cm2 sec K)')
mfprintf(fid,'\n
=========================================================================
    ')
for i=1:2
    mfprintf(fid,'\n %0.1f      %3E',u_ft(i),U(i))
end
mfprintf(fid,'\n\n\n OUTPUT Ex5.3.b');
mfprintf(fid,'\n
=========================================================================
    ')
mfprintf(fid,'\nThe Peak Radial average bed
    temperature for given Velocities' )
mfprintf(fid,'\n
=========================================================================
    ')
mfprintf(fid,'\n  u(velocity)      delta_T')
mfprintf(fid,'\n  (ft/s)           ( C )')
mfprintf(fid,'\n
=========================================================================
    ')
for i=1:2
    mfprintf(fid,'\n  %0.1f \t  \t  %0.0f',u_ft(i),
       delta_T(i))
end
mclose(fid);
//=========================================================END
    OF PROGRAM
=====================================================================
```

# Chapter 6

# Nonideal Flow

**Scilab code Exa 6.1** Power Consumption at 300 rpm speed of stirrer and blending tim

```
//Harriot P., 2003, Chemical Reactor Design (I-Edition), Marcel Dekker, Inc., USA, pp 436.
//Chapter-6 Ex6.1 Pg No.236
//Title:Power Consumption at 300 rpm,speed of stirrer and blending time
//==================================================================

clear
clc
// COMMON INPUT
D_a=0.1;
D_t=0.3;
H=0.3;
N_P=5.5;
rho=1000;
n=5;
S_f=6;//Scale up factor in diameter
P_by_V_limit=10;//Pressure per unit volume (HP/1000
gal)
n1=5;
Da_by_Dt1=D_a/D_t;
Da_by_Dt2=0.5;

//CALCULATION (Ex6.1.a)
P_unit_vol=(N_P*n^3*D_a^5)/(%pi*(1/4)*D_t^2*H);
P_thousand_gal=P_unit_vol*5.067;
t=(4/n)*(D_t/D_a)^2*(H/D_t);
P_unit_vol_new=S_f^2*P_thousand_gal;

//CALCULATION (Ex6.1.b)
n_limit=(P_by_V_limit/P_unit_vol_new)^(1/3) *n1;//Pressure per unit vol propotional to n3
t_inc_factor=n1/n_limit;//t inversely propotional to n
rotational_speed=n_limit*60;//Speed in rpm

//CALCULATION (Ex6.1.c)
n2=(Da_by_Dt1/Da_by_Dt2)^(5/3)*n_limit;
rotaional_speed=n2*60;
t1=4*(1/Da_by_Dt1)^2*(H/D_t)*(1/n_limit);
t2=4*(1/Da_by_Dt2)^2*(H/D_t)*(1/n2);

//OUTPUT (Ex6.1.a)
mprintf('\n OUTPUT Ex6.1.a');
mprintf('\n ==================================================================');
mprintf('\n The Power consumption per unit volume at 300rpm = %.2f HP/1000 gal',P_thousand_gal);
mprintf('\n\ The Power consumption scaling up sixfold in diameter = %.0f HP/1000 gal',P_unit_vol_new);


//OUTPUT (Ex6.1.b)
mprintf('\n\n\n OUTPUT Ex6.1.b');
mprintf('\n==========================================================================');
mprintf('\n The speed of the stirrer  = %.2f sec-1 or %.0f rpm',n_limit,rotational_speed);
mprintf('\n Blending time increases by factor of %.2f ',t_inc_factor);

//OUTPUT(Ex6.1.c)
mprintf('\n\n\n OUTPUT Ex6.1.c');
mprintf('\n==========================================================================');
mprintf('\n The new stirrer speed = %.2f sec-1 or %.0f rpm',n2,rotaional_speed);
mprintf('\n The new blending time  for Da/Dt ratio of 0.5 = %.1f sec',t2);

//FILE OUTPUT
fid= mopen('.\Chapter6-Ex1-Output.txt','w');
mfprintf(fid,'\n OUTPUT Ex6.1.a');
mfprintf(fid,'\n==========================================================================');
mfprintf(fid,'\n The Power consumption per unit volume at 300rpm = %.2f HP/1000 gal',P_thousand_gal);
mfprintf(fid,'\n\ The Power consumption scaling up sixfold in diameter = %.0f HP/1000 gal',P_unit_vol_new);
mfprintf(fid,'\n\n\n OUTPUT Ex6.1.b');
mfprintf(fid,'\n==========================================================================');
mfprintf(fid,'\n The speed of the stirrer  = %.2f sec-1 or %.0f rpm',n_limit,rotational_speed);
mfprintf(fid,'\n Blending time increases by factor of %.2f ',t_inc_factor);
mfprintf(fid,'\n\n\n OUTPUT Ex6.1.c');
mfprintf(fid,'\n ======================================================================== ');
mfprintf(fid,'\n The new stirrer speed = %.2f sec-1 or %.0f rpm',n2,rotaional_speed);
mfprintf(fid,'\n The new blending time  for Da/Dt ratio of 0.5 = %.1f sec',t2);
mclose(fid);
//==================================================================== END OF PROGRAM ==============================================================
//Disclaimer: In Ex6.1.c there is an arithematic error in the value of D_a/D_t. The value of  D_a/D_t should be 11.4 instead of the value reported in the textbook for D_a/D_t=11.1.
```

**Scilab code Exa 6.2** Effect of diffusion on conversion for laminar flow

```
//Harriot P., 2003, Chemical Reactor Design (I-Edition), Marcel Dekker, Inc., USA, pp 436.
//Chapter-6 Ex6.2 Pg No. 239
//Title:Effect of diffusion on conversion for laminar flow
//================================================================================================================================

clear
clc
//INPUT
D=1*10^(-2);//Diameter of pipeline (m)
R=D/2;//Radius (m)
```

```
D_m=10^(-4);//Diffusivity (m2/sec)
k=1;//Reaction rate constant (sec-1)


//CALCULATION
alpha=D_m/(k*(R^2));//Refer topic ('Diffusion in laminar flow reactors') Pg No.239


//OUTPUT
if (alpha<=0.01)
    then
    mprintf('\n The  effect of radial diffusion  on conversion can be neglected as alpha = %.0f',alpha )
else
    mprintf('\n The effect of radial diffusion makes  conversion almost as same as plug flow as alpha = %.0f',alpha)
end

//FILE OUTPUT
fid= mopen('.\Chapter6-Ex2-Output.txt','w');
if (alpha<=0.01)
    then
    mfprintf(fid,'\n The  effect of radial diffusion  on conversion can be neglected as alpha = %.0f',alpha )
else
    mfprintf(fid,'\n The effect of radial diffusion makes conversion almost as same as plug flow as alpha = %.0f',alpha)
end
mclose(fid);
//===================================================== END OF PROGRAM ===================================================
```

**Scilab code Exa 6.3** Effect of Axial dispersion and length on conversion

```
//Harriot P., 2003, Chemical Reactor Design (I-Edition), Marcel Dekker, Inc., USA, pp 436.
//Chapter-6 Ex6.3 Pg No. 248
//Title:Effect of Axial dispersion and length on conversion
//==========================================================
clear
clc
// COMMON INPUT
u=1;//Superficial velocity (cm/s)
D=2*10^(-5)//Molecular Diffusivity(cm2/s)
Re=30;//Reynolds No.
Pe_a=0.25;//Peclet No. corresponding Re No. from Fig 6.10
dp=3*(10^-1);//Particle Size (cm)
L=48;//Length of the bed (cm)
X_A=0.93;//Conversion
L_old=48;// Old bed length (cm)
L_new=L_old/2;//New bed length (cm)



//CALCULATION (Ex6.3.a)
Pe_dash=Pe_a*L/dp;//Refer Pg.No.247
one_minus_X_A=(1-X_A);
k_rho_L_by_u1=2.65;//From Fig6.12 for given  Pe_dash
X_A1=1-exp(-k_rho_L_by_u1);
//To increase the conversion more catalyst is needed
```

```
k_rho_L_by_u2=2.85;//From Fig6.12
X_A2=1-exp(-k_rho_L_by_u2);
Percentage_excess_cat_a=((k_rho_L_by_u2-k_rho_L_by_u1)/k_rho_L_by_u1)*100;

//CALCULATION(Ex6.3.b)
k_rho_L_by_u_new=k_rho_L_by_u1/2;
X_A_cal=(1-exp(-k_rho_L_by_u_new));//Calculated conversion
Pe_dash_new=Pe_dash/2;
k_rho_L_by_u_graph=1.3992;//Value obtained from Figure6.12 for the calculated conversion
Percentage_excess_cat_b=((k_rho_L_by_u_graph-k_rho_L_by_u_new)/k_rho_L_by_u_new)*100;

//OUTPUT(Ex6.3.a)
mprintf('\n OUTPUT Ex6.3.a');
mprintf('\n ==================================================================================== ');
mprintf('\n The effect of axial dispersion is significant and the percentage excess of catalyst = %.0f%%',Percentage_excess_cat_a );

//OUTPUT (Ex6.3.b)
mprintf('\n\n\n OUTPUT Ex6.3.b');
mprintf('\n ==================================================================================== ');
mprintf('\n The effect of axial dispersion is less on reducing the bed length \n The percentage excess of catalyst = %.0f%%',Percentage_excess_cat_b );

//FILE OUTPUT
fid= mopen('.\Chapter6-Ex3-Output.txt','w');
mfprintf(fid,'\n OUTPUT Ex6.3.a');
mfprintf(fid,'\n
==========================================================================
');
mfprintf(fid,'\n The effect of axial dispersion is significant and the percentage excess of catalyst = %.0f%%',Percentage_excess_cat_a );
mfprintf(fid,'\n\n\n OUTPUT Ex6.3.b');
mfprintf(fid,'\n
==========================================================================
');
mfprintf(fid,'\n The effect of axial dispersion is less on reducing the bed length \n The percentage excess of catalyst = %.0f%%',Percentage_excess_cat_b );
mclose(fid);
//=========================================================================END OF PROGRAM
==========================================================================
```

**Scilab code Exa 6.4** Conversion in packed bed for same superficial velocity

```
// Harriot P., 2003, Chemical Reactor Design (I-Edition), Marcel Dekker, Inc., USA, pp 436.
//Chapter-6 Ex6.4 Pg No.251
//Title:Conversion in packed bed for same superficial velocity
//
==========================================================================

clear
clc
//COMMON INPUT
L=2.5;//Lendth of bed(ft)
```

```
X_A=0.95;//Conversion
L_a=3;//Length of section a (ft)
L_b=2;//Length of section b (ft)
u_oa_by_u0=0.88;//Refer equation 3.64
u_ob_by_u0=1.12;
L=2.5;//(ft)


//CALCULATION (Ex6.4.a)
k_rho_L_by_u=log(1/(1-X_A));//First Order reactions
//For Section a
k_rho_L_by_u_a=k_rho_L_by_u*(L_a/L);
X_A_section_a=(1-exp(-k_rho_L_by_u_a));
//For Section b
k_rho_L_by_u_b=k_rho_L_by_u*(L_b/L);//Dimensionless Group based on ideal plug flow for first order reaction
X_A_section_b=(1-exp(-k_rho_L_by_u_b));
X_A_Ave=(X_A_section_b+X_A_section_a)/2;
Percent_X_A_Ave=X_A_Ave*100

//CALCULATION (Ex6.4.b)
k_rho_L_by_u=log(1/(1-X_A));//First Order reaction
//For Section a
k_rho_L_by_u_a=k_rho_L_by_u*(L_a/L)*(1/u_oa_by_u0);
X_A_section_a=(1-exp(-k_rho_L_by_u_a));
delP_a_by_alpha_u0_pow=L_a*(u_oa_by_u0);//Refer equation 3.64

//For Section b
k_rho_L_by_u_b=k_rho_L_by_u*(L_b/L)*(1/u_ob_by_u0);//Dimensionless Group based on ideal plug flow for first order reaction
delP_b_by_alpha_u0_pow=L_b*u_ob_by_u0;
X_A_section_b=(1-exp(-k_rho_L_by_u_b));
X_A_avg=(u_oa_by_u0*X_A_section_a+u_ob_by_u0*X_A_section_b)/2;
Percent_X_A_avg=X_A_avg*100;
```

```

//OUTPUT(Ex6.4.a)
mprintf('\n OUTPUT Ex6.4.a');
mprintf('\n===============================================================================');
mprintf('\nThe average converion when each section has same superficial velocity:%0.1f%%',Percent_X_A_Ave );

//OUTPUT(Ex6.4.b)
mprintf('\n\n\n OUTPUT Ex6.4.b');
mprintf('\n===============================================================================');
mprintf('\nThe overall conversion for different velocities:%0.1f%% ',Percent_X_A_avg );

//FILE OUTPUT
fid= mopen('.\Chapter6-Ex4-Output.txt','w');
mfprintf(fid,'\n OUTPUT Ex6.4.a');
mfprintf(fid,'\n===============================================================================');
mfprintf(fid,'\nThe average converion when each section has same superficial velocity:%0.1f%%',Percent_X_A_Ave );
mfprintf(fid,'\n\n\n OUTPUT Ex6.4.b');
mfprintf(fid,'\n===============================================================================');
mfprintf(fid,'\nThe overall conversion for different velocities:%0.1f%% ',Percent_X_A_avg );
mclose(fid);
//===========================================================================END OF PROGRAM===========================================================================
```

# Chapter 7

# Gas Liquid Reactions

**Scilab code Exa 7.1** `Overall Reaction Rate Coefficient Percent Resistance Reaction`

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition
   ) Marcel Dekker,Inc.,USA,pp 436.
//Chapter-7 Ex7.1 Pg No.260
//Title:Overall Reaction Rate Coefficient , Percent
   Resistance , Reaction Volume and Reactor Size
//
   ================================================================================

clear
clc
// COMMON INPUT
k2=8.5;//Reaction rate constant (L/mol-sec)
T=50;//Reaction condition temperature( C )
P=2;//Reaction Pressure (atm)
H_O2=8*10^4;// Solubility (atm/mol fraction)
F=17000//Feed rate (L/hr)
C_B_feed=1.6;//Feed concentration(M)
C_B_product=0.8;//Product concentration(M)
k_L_a=900;//Liquid film mass transfer coefficient(hr
-1)
k_g_a=80;//Gas film mass transfer coefficient(mol/hr L atm)
Epsilon=0.1;//Porosity
percent_inc=0.2;//Percentage excess required for reactor volume


//CALCULATION (Ex7.1.a)
H_O2_conv=H_O2*18/1000;// Convert (atm L/mole O2)
k_L_a_by_H=k_L_a/H_O2_conv;
reaction_resistance=H_O2_conv/(k2*C_B_product*(1-Epsilon)*3600);
Kg_a=1/((1/k_g_a)+(1/k_L_a_by_H)+(reaction_resistance));//Refer equation7.10
gasfilm_resistance_per=((1/k_g_a)/(1/Kg_a))*100;
liq_film_resistance_per=((1/k_L_a_by_H)/(1/Kg_a))*100;
reaction_resistance_per=((reaction_resistance)/(1/Kg_a))*100;

//CALCULATION (Ex7.1.b)
delta_C_B=C_B_feed-C_B_product;
mol_O2_needed=F*delta_C_B/4;
N_air=100;//Assuming 100 mole of feed air
f_O2=0.209;//Fraction of O2
f_N2=1-f_O2;//Fraction of N2
N_O2_in=N_air*f_O2;
N_N2_in=N_air*f_N2;
N_O2_out=N_O2_in/2;//Half of O2 fed
N_N2_out=N_N2_in;
N_air_out=N_N2_out+N_O2_out;
P_O2_out=P*(N_O2_out/N_air_out);
P_O2_in=P*(N_O2_in/N_air);
P_O2_bar=(P_O2_in-P_O2_out)/(log(P_O2_in/P_O2_out));//Log mean Pressure
volume=mol_O2_needed/(Kg_a*P_O2_bar);
reactor_vol=volume+volume*percent_inc;
```

```
volume_gal=volume*0.264;
reactor_vol_gal=reactor_vol*0.264;


//OUTPUT (Ex7.1.a)
mprintf('\n OUTPUT Ex7.1.a');
mprintf('\n==========================================================================');
mprintf('\nThe percentage  gas-film  resistance : %0.1f%%',gasfilm_resistance_per);
mprintf('\nThe percentage liquid-film resistance: %0.1f%%',liq_film_resistance_per);
mprintf('\nThe percentage chemical reaction resistance: %0.1f%%',reaction_resistance_per);

//OUTPUT (Ex7.1.b)
mprintf('\n\n\n OUTPUT Ex7.1.b');
mprintf('\n==========================================================================');
mprintf('\n Reaction volume  calculated : %0.0f L ',volume );
mprintf('\n Reactor size to be chosen : %0.0f L',reactor_vol);


// FILE OUTPUT
fid= mopen('.\Chapter7-Ex1-Output.txt','w');
mfprintf(fid,'\n OUTPUT Ex7.1.a');
mfprintf(fid,'\n==========================================================================');
mfprintf(fid,'\nThe percentage  gas-film  resistance : %0.1f%%',gasfilm_resistance_per);
mfprintf(fid,'\nThe percentage liquid-film resistance: %0.1f%%',liq_film_resistance_per);
mfprintf(fid,'\nThe percentage chemical reaction
resistance: %0.1f%%',reaction_resistance_per);
mfprintf(fid,'\n\n\n OUTPUT Ex7.1.b');
mfprintf(fid,'\n===================================================================================================');
mfprintf(fid,'\n Reaction volume  calculated : %0.0f L ',volume );
mfprintf(fid,'\n Reactor size to be chosen : %0.0f L ',reactor_vol);
mclose(fid);
//==================================================================================== END OF PROGRAM ==========================================================================================
```

**Scilab code Exa 7.2** The gradient for B in the liquid film

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc. USA,pp 436.
//Chapter-7 Ex7.2 Pg No.270
//Title:The gradient for B in the liquid film
//==============================================================================================================
clear
clc
//INPUT
C_B0_by_C_Ai=40;
D_A_by_D_B=1.2;
sqrt_M=10;
phi=sqrt_M;//Assume the gradient for A is the same as when the gradient for B is negligible
```

```
eff_diff_distA_by_xL=(1/phi);

//CALCULATION
eff_diff_distB_by_xL=(1-eff_diff_distA_by_xL);
CB0_minus_CBbar_by_CB0=D_A_by_D_B*(1/C_B0_by_C_Ai)*(eff_diff_distB_by_xL/eff_diff_distA_by_xL);
C_Bbar_by_C_B0=(1-CB0_minus_CBbar_by_CB0);
sqrt_kC_B=sqrt(C_Bbar_by_C_B0);
phi_corrected=phi*sqrt_kC_B;
Percent_change=((phi-phi_corrected)/(phi))*100;

//OUTPUT
mprintf('\n  Percentage Decrease in Rate :%0.0f%% ',Percent_change);
mprintf('\n The decrease in rate is significant ,hence the gradient for B is significant in liquid film');
fid= mopen('.\Chapter7-Ex2-Output.txt','w');
mfprintf(fid,'\n  Percentage Decrease in Rate :%0.0f%% ',Percent_change);
mfprintf(fid,'\n The decrease in rate is significant ,hence the gradient for B is significant in liquid film');
mclose(fid);
//==========================END OF PROGRAM==========================
```

**Scilab code Exa 7.3** Overall mass transfer coefficient and percent resistance

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc.,USA,pp 436
```

```
//Chapter-7 Ex7.3 Pg No.274
//Title:Overall mass transfer coefficient and percent resistance
//==========================================================================
clear
clc
//INPUT
k2=8500;//(L/mol sec) at 25  C
kg_a= 7.4 //(mol/hr ft3 atm)
k_star_L_a=32;//(hr-1)
a=34;//(ft2/ft3)
H_CO2=1.9*10^(3);//(atm/m f) Henry's Constant
D_CO2=2*10^(-5);//(cm2/sec)
D_OH=2.8*10^(-5);//(cm2/sec)
P_CO2_in=0.04;//(atm)
P_CO2_out=0.004;//(atm)
Caustic_conc=[0.5 0.75];//Cocentration on both the ends of the column bottom and top(M)
n=2;
M_H2O=18;//Molecular Weight
H_H2O=62.3;//(g/ft3) Henry's Constant
H_H2O_dash=H_H2O/M_H2O;//Henry's Constant converted into consistent units with kg_a


//CALCULATION
C_Ai=P_CO2_in/H_CO2*(1000/18);
k_star_L=(k_star_L_a/(a*3600))*(30.5);
H_CO2_dash=H_CO2*(1/H_H2O_dash);
for i=1:2
Phi_a(i)=(1+(Caustic_conc(i)/(n*C_Ai))*(D_OH/D_CO2));//Refer equation7.51
sqrt_M(i)=sqrt(k2*Caustic_conc(i)*D_CO2)/k_star_L;
Phi(i)=sqrt_M(i);//Refer fig 7.7
K_ga(i)=(1/((1/kg_a)+(H_CO2_dash/(Phi(i)*k_star_L_a))));//Overall Mass transfer coefficient
```

```
Percent_resis_gasfilm(i)=(K_ga(i)/kg_a)*100;
end

//OUTPUT
mprintf('\n \t\t\t\t\t\t\tTop\t   Bottom');
mprintf('\n Overall mass transfer coefficient (mol/hr ft3 atm): %0.1f\t %0.1f',K_ga(1),K_ga(2));
mprintf('\n Percenage resistance in gas film:                    %0.0f%%\t        %0.0f%% ',Percent_resis_gasfilm(1) ,Percent_resis_gasfilm(2) );

//FILE OUTPUT
fid= mopen('.\Chapter7-Ex3-Output.txt','w');
mfprintf(fid,'\n \t\t\t\t\t\t\tTop\t   Bottom');
mfprintf(fid,'\n Overall mass transfer coefficient (mol/hr ft3 atm): %0.1f\t %0.1f',K_ga(1),K_ga(2));
mfprintf(fid,'\n Percenage resistance in gas film:                    %0.0f%%\t      %0.0f%% ',Percent_resis_gasfilm(1) ,Percent_resis_gasfilm(2) );
mclose(fid);
//
   ==================================================================================
   END OF PROGRAM
   ==================================================================================
```

**Scilab code Exa 7.4** Local selectivity due to mass transfer limitations

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc.,USA,pp 436
//Chapter-7 Ex7.4 Pg No.279
```

```
//Title:Local selectivity due to mass transfer limitations
//==========================================================================
clear
clc
//INPUT
C_Ai=0.02;//(M)
C_B0=3;//(M)
D_A=10^(-5);//(cm2/sec)
D_B=D_A;//(cm2/sec)
D_C=D_B;//(cm2/sec)
k_1=10^(4);//(L/mol sec)
k_star_l=0.015;//(cm/sec)
n=1;
C_c0=[0 1.4];
X=[0 0.5]// Conversion
Phi=[33 23];//From figure 7.7


//CALCULATION
k_2=0.09*k_1;
for i=1:2
    C_B(i)=(1-X(i))*C_B0;
sqrt_M(i)=sqrt(C_B(i)*k_1*D_A)/k_star_l;
Phi_a(i)=(1+(C_B(i)/(n*C_Ai))*(D_B/D_A));//Refer equation 7.51
C_Bbar_by_C_B(i)=(Phi(i)/sqrt_M(i))^2;//Refer equation 7.59
delta_C_B(i)=(1-C_Bbar_by_C_B(i))*C_B(i);//Refer equation 7.60
delta_C_c(i)=delta_C_B(i);
C_cbar(i)=delta_C_c(i)+C_c0(i);
C_Bbar(i)=C_Bbar_by_C_B(i)*(C_B(i));
S(i)=(1-(k_2*C_cbar(i)/(C_Bbar(i)*k_1)))*100;//Refer equation 7.56
end
```

```

//OUTPUT
mprintf('\n\tLocal selectivity due to mass transfer limitations ');
mprintf('\n\tThe local selectivity for Zero Conversion : %0.0f%%',S(1));
mprintf('\n\tThe local selectivity for 50%% Conversion : %0.0f%%',S(2));

//FILE OUTPUT
fid= mopen('.\Chapter7-Ex4-Output.txt','w');
mfprintf(fid,'\n\tLocal selectivity due to mass transfer limitations ');
mfprintf(fid,'\n\tThe local selectivity for Zero Conversion is %0.0f%%',S(1));
mfprintf(fid,'\n\tThe local selectivity for 50%% Conversion is %0.0f%%',S(2));
mclose(fid);
//==========================================================
END OF PROGRAM
===========================================================
```

**Scilab code Exa 7.5** Maximum rate of CO absorption and Dimensions of Bubble Column

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc.,USA,pp 436
//Chapter-7 Ex7.5 Pg No.293
//Title:Maximum rate of CO absorption  and Dimensions of Bubble Column Reactor
//==========================================================
clear
clc
// COMMON INPUT
P_dash=5;//Partial pressure of acetic acid (atm)
P_total=20;//Total Pressure (atm)
myu=0.19;// Viscosity of acetic acid
T_C=180;//Temperature in ( C )
T_K=T_C+273;//Temperature in (K)
sigma_20=28;//Surface Tension(Dynes/cm) at 20 ( C )
sigma_180=20;//Surface Tension (Dynes/cm)at 180 ( C )
M_CO=28;//Molecular weight of CO
M_B=60.05;//Molecular weight acetic acid
V_A= 30.7;//Molar volume
S_CO=7*10^(-3);//Solubility of CO (mol/L atm)
f_CO=0.75;//Fraction of CO in feed
f_acetic_acid=1-f_CO;//Fraction of Acetic acid
R=82.056*(10^-3);//( cm3 atm /  K    mol  )
rho_air=1.21;//(kg/m3)density of air at 20 ( C )
sigma_H2O=72;//Surface tension (Dynes/cm)
myu_H2O=1;//Viscosity of water
k_L_a_air_water=0.051;//(sec -1)
D_O2_water=2.4*(10^-5);//(cm2/sec)diffusivity for oxygen in waterat 20( C )
Conc_Rh=4*10^(-3);//Concentration of Rohdium(M)
Conc_CH3I=1;//Concentration of Methyl Iodide(M)
F_product_acetic_acid=0.1;// Rate of acetic acid produced (kmol/sec)
f_CO_reacted=0.8;//80% of CO reacted
u_g=0.1;//(m/sec)
Epsilon_air_water_new=0.07;//At velocity  3(cm/sec)
Epsilon_air_water_old= 0.12;//At velocity 6(cm/sec)
u_g_c=5*(10^(-2));//Gas Velocity  Ex7.5.c(m/sec)



//CALCUATION (Ex7.5.a)
```

```
D_CO=(7.4*10^(-8)*M_B^(1/2)*T_K)/(myu*V_A^(0.6));//Diffusivity of CO (WilkeChang equation Eq4.17)
M_ave=f_CO*M_CO+M_B*f_acetic_acid;//Average Molecular weight
rho_g=M_ave*P_total/(R*T_K);//From ideal gas law
epsilon_air_water= 0.12;//At velocity 6(cm/sec)
epsilon=epsilon_air_water*(sigma_H2O/sigma_180)^(0.4)*(myu/myu_H2O)^(0.2)*(rho_g/rho_air)^(0.2);//From equation 7.64
u_G=6;//From figure 7.12(cm/sec)
k_L_a=k_L_a_air_water*(D_CO/D_O2_water)^(0.5)*(epsilon/epsilon_air_water);//From equation 7.69
P_CO=P_total-P_dash;
C_CO_Star=S_CO*P_CO;
r_max=C_CO_Star*k_L_a;//Rate of CO absorption at 15 atm
r_test=158.8*(10^(6))*exp(-8684/T_K)*(Conc_Rh)*(Conc_CH3I);//Kinetic rate at 180 ( C )

//CALCULATION(Ex7.5.b)
F_feed_CO=F_product_acetic_acid/f_CO_reacted;//Rate of flow of CO (kmol/sec)
F_total=F_feed_CO/f_CO;
Q=F_total*R*T_K/(P_total);
S=Q/u_g;
D_t=sqrt(4*S/%pi);
r_test_b=(158.8*(10^(6))*exp(-8684/T_K)*(Conc_Rh)*(Conc_CH3I))*(10^(-3));//Kinetic rate at 180 ( C )
liquid_vol= (F_product_acetic_acid/r_test_b)*(10^(-3));//liquid volume (m3)
h0=liquid_vol/S;//clear liquid
h=h0/(1-epsilon);//aerated liquid

//CALCULATION(Ex7.5.c)
Q=F_total*R*T_K/(P_total);
S=Q/u_g_c;
D_t_c=sqrt(4*S/%pi);
Epsilon_new=(Epsilon_air_water_new/
    Epsilon_air_water_old)*epsilon;
liquid_vol= (F_product_acetic_acid/r_test_b)*(10^(-3));//liquid volume (m3)
h0=liquid_vol/S;//clear liquid
h_new=h0/(1-Epsilon_new);//aerated liquid

//OUTPUT (Ex7.5.a)
mprintf('\n OUTPUT Ex7.5.a');
mprintf('\n========================================================');
mprintf('\n\tThe maximum rate of CO absorption at 15 atm : %f (mol/L s)',r_max);
mprintf('\n\tThe kinetic rate of CO absorption at 180( C ) : %f (mol/L s)',r_test);
mprintf('\n\tThe predicted value of k_L_a : %0.2f (s-1)',k_L_a);

//OUTPUT (Ex7.5.b)
mprintf('\n\n\n OUTPUT Ex7.5.b');
mprintf('\n========================================================');
mprintf('\n\tThe Dimensions of the reactor are ');
mprintf('\n\tDiameter:%0.0f m',D_t);
mprintf('\n\tHeight:%0.2f m',h);

//OUTPUT (Ex7.5.c)
mprintf('\n\n\n OUTPUT Ex7.5.c');
mprintf('\n========================================================');
mprintf('\n\tThe new dimensions of the reactor');
mprintf('\n\tDiameter:%0.1f m',D_t_c);
mprintf('\n\tHeight:%0.1f m',h_new);

//FILE OUTPUT
fid= mopen('.\Chapter7-Ex5-Output.txt','w');
```

```
mfprintf(fid,'\n OUTPUT Ex7.5.a');
mfprintf(fid,'\n============================================================');
mfprintf(fid,'\n\tThe maximum rate of CO absorption at 15 atm : %f (mol/L s)',r_max);
mfprintf(fid,'\n\tThe kinetic rate of CO absorption at 180( C ) : %f (mol/L s)',r_test);
mfprintf(fid,'\n\tThe predicted value of k_L_a : %0.2f (s-1)',k_L_a);
mfprintf(fid,'\n\n\n OUTPUT Ex7.5.b');
mfprintf(fid,'\n============================================================');
mfprintf(fid,'\n\tThe Dimensions of the reactor are');
mfprintf(fid,'\n\tDiameter:%0.0f m',D_t);
mfprintf(fid,'\n\tHeight:%0.2f m',h);
mfprintf(fid,'\n\n\n OUTPUT Ex7.5.c');
mfprintf(fid,'\n============================================================');
mfprintf(fid,'\n\tThe new dimensions of the reactor');
mfprintf(fid,'\n\tDiameter:%0.1f m',D_t_c);
mfprintf(fid,'\n\tHeight:%0.1f m',h_new);
mclose(fid);

//==================================================END OF PROGRAM============================================================
```

**Scilab code Exa 7.6** Fraction of O2 Power of agitator kLa and average dissolved oxy

```
//Harriot P,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc., USA,pp 436.
//Chapter-7 Ex7.6 Pg No.300
//Title:Fraction of O2,Power of agitator , k_L_a and average dissolved oxygen concentration.
//
clear
clc
// COMMON INPUT
Vol_reactor=200;//Volume of reactor (m3)
D=4;//Diameter of reactor (m)
depth=12;//Depth of reactor (m)
u_g=3;//Superficial velocity (cm/sec)
T_C=30;//Temperature ( C )
T_K=273+T_C;//Temperature  (K)
f_O2=0.21;//Fraction of O2 in air
myu_soln=1.5*(10^(-3));//Viscosity of solution (Pa sec)
R=0.08206;//Gas constant ( m 3 atm /  K  kmol)
r_O2_peak=45*(10^(-3));//Flow rate of O2 at peak demand
Da_by_Dt=(1/3);
Da=1.333;//(m)
N=120;//(rpm)
N_conv=(N/60);//(sec-1)
Press_top=1;//Pressure at the top of the vessel (atm)
rho=1000;//Density of water (kg/m3)
ug_sup1=3*(10^(-2));//based on 30( C ) and 1 (atm)
V=151;//Volume of solution calculated Ex7.6.a (m3)
ug_sup1=3*(10^(-2));//based on 30( C ) and 1 atm.
Press_top=1;//Pressure at the top of the vessel (atm)
Press_bottom=2;//From Ex7.6.c
```

```
ug_sup2=ug_sup1/Press_bottom;// at 2atm superficial velocity (cm/sec)
ug_ave=(ug_sup1+ug_sup2)/2;//Average superficial velocity (cm/sec)
depth=12;//Depth of reactor (m)
one_atm_water=10.3;//1 atm pressure corresponds to 10.3 (m) height of water
k_H_O2=5.2*10^(4)// Henery's law constant  for O2 in water for O2 (atm/mol fraction)
M_O2=32;//Molecular weight of O2
M_H2O=18;//Molecular weight of water
C_O2_critical=1*10^(-3);//Critical O2 Concentration (g/L)
percent_reduction=40/100;//Mass transfer coefficient in the upper region of the reactor is 40% less than the average
kLa_soln=0.22;//Value calculated in Ex7.6.d
r_conv=1.25*10^(-5);//Rate at peak O2 demand (mol/L sec)
depth=12;//Depth of reactor (m)


//CALCULATION (Ex7.6.a )
S=%pi*(D^2)/4;//Cross section area (m2)
V=S*depth;//Volume of solution(m3)
F_air=(S*u_g*(10^(-2))*3600)/(R*(10^(-3))*T_K);
F_O2=f_O2*F_air;//Feed rate of O2 (mol/hr)
F_O2_used=r_O2_peak*V*(10^(3));//O2 used for aerobic fermentation (mol/hr)
F_O2_left=F_O2-F_O2_used;//O2 left after aerobic fermentation(mol/hr)
f_O2_exitgas=F_O2_left/F_air;//Fraction of O2 in exit gas
Percent_O2_exitgas=(f_O2_exitgas)*(100);
Frac_O2_used=((f_O2-f_O2_exitgas)/f_O2);

//CALCULATION (Ex7.6.b )
Re=(rho*N_conv*Da^2)/myu_soln;
```

```
N_p=6;//For a standard turbine
N_p_pitched=1.7;//For a pitched-blade turbine
P0=(N_p*rho*(N_conv^3)*(Da^5))*(10^(-3));//Refer equation 7.73 (kW)
//If the turbine is 2 m from the bottom, or 10 m below the surface,the pressure is about 2 atm since 1atm= 10.3 m water
Press_bottom=2
ug_sup2=ug_sup1/Press_bottom;
Q=ug_sup2*S;
N_Ae=Q/(N_conv*(Da^3));
Pg_by_P0=0.55;//From figure 7.15 based on N_Ae value  calculated
Pg=Pg_by_P0*P0;//When aerated
P0_pitched=(N_p_pitched/N_p)*P0;
Pg_by_P0_pitched=0.8;//Solution reaching the upper stirrers is already aerated
Pg_pitched=Pg_by_P0_pitched*P0_pitched;
Tot_Pow_no_air=P0+Press_bottom*P0_pitched;//Total power when no air is presented
Tot_Pow_aerated=Pg+Press_bottom*Pg_pitched;//Total power when it is aerated

//CALCULATION (Ex7.6.c )
P_by_V_ave=Tot_Pow_aerated/V;
kLa_O2_sulfite=0.32;//Using figure7.16 based on ave(P/V) value and ug_average value
kLa_soln=0.7*kLa_O2_sulfite;//kLa for this solution is 70% of the value for oxygen absorption in sodium sulfite (sec-1)
y_O2=0.086;//If gas is backmixed
depth_ave=depth/2;
Press_ave=(Press_top+(depth_ave/one_atm_water));//Pressure at average depth (atm)
C_O2_star=(Press_ave*y_O2/k_H_O2)*(1000/M_H2O);//Conversion (mol/L)
r_conv=r_O2_peak/3600;//Rate at peak O2 demand (mol/L sec)
```

```
C_ave=(C_O2_star-(r_conv/kLa_soln))
C_ave_conv=C_ave*M_O2*1000;//Converted value of O2 concentration in(mg/L)

//CALCULATION (Ex7.6.d)
depth_ave=depth/2;
Press_ave=(Press_top+(depth_ave/one_atm_water));//Pressure at average depth (atm)
kLa_soln_reduced=kLa_soln*(1-percent_reduction);
C_star_minus_C=r_conv/kLa_soln_reduced;
C_O2_new=(C_O2_star-(C_star_minus_C));
C_O2_new_conv=C_O2_new*M_O2*1000;//Converted value of O2 concentration in(mg/L)
C_O2_star_new=C_O2_star/Press_ave;

//OUTPUT (Ex7.6.a)
mprintf('\n OUTPUT Ex7.6.a');
mprintf('\n==================================================================');
mprintf('\nAt the peak demand, fraction of the oxygen supplied = %.3f ',Frac_O2_used);

//OUTPUT(Ex7.6.b )
mprintf('\n\n\n OUTPUT Ex7.6.b');
mprintf('\n==================================================================');
mprintf('\nThe total power required for the agitator before the air is turned on: %0.0f kW',Tot_Pow_no_air);
mprintf('\nThe total power required for the agitator after the air is turned on: %0.0f kW',Tot_Pow_aerated);

//OUTPUT (Ex7.6.c )
mprintf('\n\n\n OUTPUT Ex7.6.c');
mprintf('\n
========================================================================
');
mprintf('\nThe calculated value of kLa (mass transfer coefficient) of solution:%0.2f (sec-1)',kLa_soln);
mprintf('\nThe calculated value of average dissolved O2 concentration: %0.2f (mg/L)',C_ave_conv);

 //OUTPUT (Ex7.6.d)
 mprintf('\n\n\n OUTPUT Ex7.6.d');
mprintf('\n
========================================================================
');
 mprintf('\nThe new calculated value of average dissolved O2 concentration  %0.2f (mg/L)',C_O2_new_conv);
 if(C_star_minus_C>C_O2_star_new)
     mprintf('\nThe reactor is operated above critical O2 concentration ');
 else
     mprintf('\nThe reactor should be operated at higher air rate otherwise C_O2 would drop to zero')
 end
 // FILE OUTPUT
fid= mopen('.\Chapter7-Ex6-Output.txt','w');
mfprintf(fid,'\n OUTPUT Ex7.6.a');
mfprintf(fid,'\n
========================================================================
');
mfprintf(fid,'\nAt the peak demand, fraction of the oxygen supplied = %.3f ',Frac_O2_used);
mfprintf(fid,'\n\n\n OUTPUT Ex7.6.b');
mfprintf(fid,'\n
========================================================================
');
mfprintf(fid,'\nThe total power required for the agitator before the air is turned on: %0.0f kW',
   Tot_Pow_no_air);
mfprintf(fid,'\nThe total power required for the
   agitator after the air is turned on: %0.0f kW',
   Tot_Pow_aerated);
mfprintf(fid,'\n\n\n OUTPUT Ex7.6.c');
mfprintf(fid,'\n
  ==========================================================================
   ');
mfprintf(fid,'\nThe calculated value of kLa (mass
   transfer coefficient) of solution:%0.2f (sec-1)',
   kLa_soln);
mfprintf(fid,'\nThe calculated value of average
   dissolved O2 concentration: %0.2f (mg/L)',
   C_ave_conv);
mfprintf(fid,'\n\n\n OUTPUT Ex7.6.d');
mfprintf(fid,'\n
  ==========================================================================
   ');
mfprintf(fid,'\nThe new calculated value of average
   dissolved O2 concentration  %0.2f (mg/L)',
   C_O2_new_conv);
 if(C_star_minus_C>C_O2_star_new)
     mfprintf(fid,'\nThe reactor is operated above
        critical O2 concentration ');
 else
     mfprintf(fid,'\nThe reactor should be operated
        at higher air rate otherwise C_O2 would drop
         to zero')
 end
 mclose(fid);
//
  =================================================================
   END OF PROGRAM
  ====================================================================
```

**Scilab code Exa 7.7** Apparent value of kLa regime of operation and selectivity depe

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc.,USA,pp 436.
//Chapter-7 Ex7.7 Pg No.304
//Title:Apparent value of kLa, regime of operation and selectivity dependency on gas mixing
//===================================================================================
clear
clc
//INPUT
Vol_reactor=35;//Volume of reactor(L)
No_reactor=3;//No. of reactor
T_C=155;//Operating Temperature ( C )
T_ref=273;//Reference Temperature ( C )
T_K= T_C+T_ref;//Operating Temperature (K)
P=8.2;//Operating Pressure (atm)
X_conversion=9.5*10^(-2);//Conversion
S=73*10^(-2);//Selectivity
M_cyclohexane=84.16;//Molecular weight of cyclohexane
F_cyclohexane=100;//Feed rate of cyclohexane (L/hr)
F_air=9.9;//Feed rate of air (nm3/hr)
f_O2_air=0.21;//Fraction of O2 in air
V_ref=22400;//Reference volume at STP(cm3/mol)
y_O2=0.002;//O2 in vent gas
f_O2_consumed=0.99;//Fraction of O2 Consumed
rho_cyclohexane=0.779;//Density of cyclohexane at 20 ( C )
main_pdt_ratio=3/2;
```

```
by_pdt_ratio=(1-main_pdt_ratio);
stoi_rxn_O2=[0.5 1];
rho_M=0.650;//Density of Cyclohexane at 155 ( C )
P_dash=5.8;//Vapour Pressure of cyclohexane at 155 (
    C )
D_reactor=30;//Diameter of reactor (cm)
h_reactor=50;//Height of reactor (cm)
myu_20=0.98;//(cp) Viscosity at 20( C )
myu_155=0.2// (cp) Viscosity at 155( C )
x_O2=6.38*(10^(-6));//Mol fraction of O2
D_B_by_D_A=0.5;//Assumed value (refer Ex7.7)
Phi=20;//Refer Fig. 7.7
n=1/(0.7);


//CALCULATION (Ex7.7.a )
F_O2=(F_air*10^(6)*f_O2_air)/(3600*V_ref);
delta_N_O2=F_O2*f_O2_consumed;
F_C6=(F_cyclohexane*10^(3)*rho_cyclohexane)/(3600*
   M_cyclohexane)
F_prdts=F_C6*X_conversion*S;
F_O2_prdts=F_prdts*(main_pdt_ratio*stoi_rxn_O2(1)+
   by_pdt_ratio*stoi_rxn_O2(2));
F_O2_remain_used=delta_N_O2-F_O2_prdts;
F_O2_prdts_conver=F_O2_prdts/(F_C6*X_conversion*S);
F_O2_remain_used_conver=F_O2_remain_used/(F_C6*
   X_conversion*(1-S));
X_O2=10^(0.366*log10(T_K)-3.8385);//O2 solubility
   from Wild et al. [37]:
PO2_plus_PN2=P-P_dash;
P_O2=y_O2*PO2_plus_PN2;
x_O2=P_O2*X_O2;//Mol fraction of O2
C_M=rho_M*10^(3)/M_cyclohexane;
C_O2_star=C_M*x_O2;

//Assume each reactor has 30 L solution
V_soln_n=30;//Volume of solution in each reactor
apparent_kLa=(delta_N_O2)/(V_soln_n*No_reactor*
C_O2_star);
F_total=(F_air*10^(6)/3600)*(T_K/T_ref)*(8.2/2.4)*(1/8.2);//The total vapor flow is 8.2/2.4 times the air flow
CSA_reactor=%pi*(D_reactor^2)/4;
u_g=F_total/(CSA_reactor*No_reactor);
//Calculation for predicted value of kLa
kLa_20=0.16;//From Figure 7.16, for O 2 C6H12 at 20 ( C ), 2 cm/sec, 5 kW/m3
T_data=20+T_ref;//Temperature at which data is taken from the table
D_155_by_D_20=(T_K/T_data)*(myu_20/myu_155);
Predicted_kLa=kLa_20*(D_155_by_D_20^(0.5))*(u_g/2)^(0.5);

//CALCULATION (Ex7.7.b )
C_M=rho_M*10^(3)/M_cyclohexane;
C_B0=(1-X_conversion)*C_M;
C_Ai=C_M*x_O2;
Phi_a=(1+(C_B0/(C_Ai*n))*(D_B_by_D_A)^(0.5));
ratio=Phi_a/Phi;

//OUTPUT (Ex7.7.a )
mprintf('\n OUTPUT Ex7.7.a');
mprintf('\n==========================================================');
mprintf('\nThe value of apparent kLa: %0.2f (sec-1)',apparent_kLa);
mprintf('\n The value of predicted kLa: %0.2f (sec-1)',Predicted_kLa);
if (apparent_kLa>Predicted_kLa)
    mprintf('\nThe absorption of oxygen is greatly enhanced by chemical reactions in the liquid film')
    mprintf('\nThe kinetics can be approximated by a first-order expression,the reaction would fall in the pseudo-first-order regime,\
nwhere the rate varies with the square root of the oxygen diffusivity and the rate constant.')
end

//OUTPUT (Ex7.7.b )
mprintf('\n\n\n OUTPUT Ex7.7.b');
mprintf('\n========================================================================');
mprintf('\nThe value of Phi (enhancement factor) %0.4E ',Phi_a);
mprintf('\nThe value of ratio Phi_a_by_Phi:%0.1E',ratio);
mprintf('\nFrom the ratio value Phi_a is greater than Phi hence there is no significant gradient for cyclohexane');

// FILE OUTPUT
fid= mopen('.\Chapter7-Ex7-Output.txt','w');
mfprintf(fid,'\n OUTPUT Ex7.7.a');
mfprintf(fid,'\n========================================================================');
mfprintf(fid,'\nThe value of apparent kLa: %0.2f (sec-1)',apparent_kLa);
mfprintf(fid,'\n The value of predicted kLa: %0.2f (sec-1)',Predicted_kLa);
if (apparent_kLa>Predicted_kLa)
    mfprintf(fid,'\nThe absorption of oxygen is greatly enhanced by chemical reactions in the liquid film')
    mfprintf(fid,'\nThe kinetics can be approximated by a first-order expression,the reaction would fall in the pseudo-first-order regime,\nwhere the rate varies with the square root of the oxygen diffusivity and the rate constant.')
```

```
end
mfprintf(fid,'\n\n\n OUTPUT Ex7.7.b');
mfprintf(fid,'\n======================================================================================================');
mfprintf(fid,'\nThe value of Phi (enhancement factor) %0.4E ',Phi_a);
mfprintf(fid,'\nThe value of ratio Phi_a_by_Phi:%0.1E',ratio);
mfprintf(fid,'\nFrom the ratio value Phi_a is greater than Phi hence there is no significant gradient for cyclohexane');
mclose(fid);
//======================================================================================================END OF PROGRAM==================================================================================
```

# Chapter 8

# Multiphase Reactors

**Scilab code Exa 8.1** Gas absorption coefficient and fraction of overall resistance

```
//Harriot P., 2003, Chemical Reactor Design (I-Edition), Marcel Dekker, Inc., USA, pp 436.
//Chapter-8 Ex8.1 Pg No. 323
//Title:Gas absorption coefficient and fraction of overall resistance
//
clear
clc
//INPUT
rho_oil=0.8;//Density of oil (g/cm3)
IV_init=130;//Iodine Value initial
IV_final=80;//Iodine Value final
P=45;//Pressure of system (psig)
T_C=204;// Temperature of system ( C )
t_run=[26 17];//Time required for hydrogenation run 2;
frac_Ni=[0.005 0.0125]//Fraction of Nickel used for
```

```
different run

//CALCULATION
r_ave=((IV_init -IV_final))*(0.039*rho_oil)*(1/60).*(t_run.^(-1));//Relationship between Iodine value and Hydrogen consumption (mol- H2/ L sec)
H_H2= 4*10^(-3);//Solubility of H2 from Fig8.4 Pg No.322
P_H2=(P/14.7)+1;//Absolute Pressure in (atm)
C_H2=P_H2 *H_H2;
Ci_by_r=C_H2.*(r_ave.^(-1));
Coeff_R_cat=frac_Ni.^(-1);
equation=[ones(1,2);Coeff_R_cat]//Simultaneous Equation
Resistance= Ci_by_r*inv(equation);
Gas_abs_resistance=(Resistance(1)*100 ).*(Ci_by_r.^(-1));
Gas_abs_coefficient=(1/Resistance(1));

//OUTPUT
mprintf('\nThe Gas absorption coefficient is %f sec-1',Gas_abs_coefficient);
mprintf('\n The Fraction of overall resistance due to gas absorption\n  Run 1 %0.0f%% \n  Run 2 %0.0f%%',Gas_abs_resistance(1),Gas_abs_resistance(2));

//FILE OUTPUT
fid= mopen('.\Chapter8-Ex1-Output.txt','w');
mfprintf(fid,'\nThe Gas absorption coefficient is %f sec-1',Gas_abs_coefficient);
mfprintf(fid,'\n The Fraction of overall resistance due to gas absorption\n  Run 1 %0.0f%% \n  Run 2 %0.0f%%',Gas_abs_resistance(1),Gas_abs_resistance(2));
mclose(fid);
//
```

END OF PROGRAM

**Scilab code Exa 8.2** External Mass Transfer resistance

```
//Harriot P., 2003, Chemical Reactor Design (I-Edition), Marcel Dekker, Inc., USA, pp 436.
//Chapter-8 Ex8.2 Pg No. 329
//Title:External Mass Transfer resistance
//

clear
clc
//INPUT
Chi=1.9;
M_A=2;//Molecular weight of Hydrogen
M_B=32;//Molecular weight of methanol
rho=0.79;//Density of methanol
myu=0.52;//Viscosity of methanol (cP)
V_A=14.3//Molar volume H2
T_C=30;//Operating Temperature( C )
T_K=273+T_C//Temperature (K)
Epsilon=0.4;//Porosity
rho_cat_dry=1.2;//Density of dry catalyst (g/cm3)
rho_s=2;//Solid density
g=9.8// Acceleration due to gravity(m/s2)
d_p=10^(-3);//Size of catalyst (cm)
lambda=1.3;//From equation 8.4 Pg. No. 317
r_vol=2.4;//Measured rate (L/min)
V_mol=22.4;//(L/mol) assuming ideal gas
C_H2=4.1*10^(-3);//From Figure 8.3 (mol/L)  Pg. No.
```

```
321


//CALCULATION
//Assume D_H2 is three times the value given by the Wilke Chang Equation
D_H2=3*(7.4*(10^(-8))*(Chi*M_B)^(0.5)*T_K)/(myu*(V_A)^0.6)
Sc=myu*10^-2/(rho*D_H2);
rho_cat_methanol=(1-Epsilon)*rho_s+Epsilon*rho;
delta_rho=rho_cat_methanol-rho;
v_t=(g*10*(d_p)^2*delta_rho)/(18*myu*10^-2);// From Stoke's Law
Re=rho*v_t*d_p/(myu*10^-2);
Sh_star=2+0.6*(Re)^(0.5)*(Sc^(1/3));//Refer equation 8.9  Pg.No.325
kc_star=Sh_star*D_H2/d_p;
kc=2*kc_star;//With vigorous agitation
a_c=6*lambda/(d_p*rho_cat_dry);//From Equation 8.4 Pg. No. 317
r_mol=r_vol/(22.4*60);//
delta_C_ext=r_mol*10^3/(kc*a_c);
percent_ext_resistance=(delta_C_ext/C_H2)*100;

//OUTPUT
mprintf('\nThe external mass transfer resistance is about %0.0f%% of overall resistance',percent_ext_resistance);
mprintf('\n The external mass transfer resistance is barely significant');

//FILE OUTPUT
fid= mopen('.\Chapter8-Ex2-Output.txt','w');
mfprintf(fid,'\nThe external mass transfer resistance is about %0.0f%% of overall resistance',percent_ext_resistance);
mfprintf(fid,'\n The external mass transfer resistance is barely significant');
```

```
mclose(fid);
//========================================================================END OF PROGRAM==========================================================
```

**Scilab code Exa 8.3** Apparent rate constant and consistency

```
//Harriot P., 2003, Chemical Reactor Design (I-Edition), Marcel Dekker, Inc., USA, pp 436.
//Chapter-8 Ex8.3 Pg No.
//Title:Apparent rate constant and consistency
//==================================================================================================================

clear
clc
// COMMON INPUT
LHSV_inv=[0.75 1.39];//Refer table 8.2 Test Results (Liquid Hourly Space Velocity)
X_S=[0.77 0.83];//Refer table 8.2 Percentage Sulphur removal
T_C=365;//Operating Temperature ( C )
rho=0.64;//Density of Sulphur Compounds (g/cm3)
myu=0.5;//Viscosity(cP)
T_K=273+T_C;//Temperature (K)
M_B=374;//For CHS compounds(Refer table8.1)
V_A=M_B/0.6;//Molar volume
Chi=1;
Epsilon_by_tau=0.1;
D_pore_by_D_bulk=0.5;//Hinderance due to large molecules
```

```
epsilon_holdup=0.6;// Assuming bed consists 60% catalyst
k_app_rhob=1.96//Refer Ex8.3.a Run 1
eta=0.74;
R=0.095;//Size of particle
C_H2_incorrect=0.48;//Solubility of H2 at 56 atm
P_incorrect=56;//Incorrect Pressure
P_correct=65;//Correct Pressure
m_feed=640;// Concentration of Feed (g/L);
percent_S=2.04;//Percentage of Sulphur
MW_S=32;//Molecular weight of Sulphur
N_H2=1.5;//Moles of H2
V_H2=14.3;//Solubility of Hydrogen

//CALCULATION (Ex8.3.a)
for i=1:2
    kapp_rhob(i)=log((1/(1-X_S(i))))*(1/LHSV_inv(i));//Refer Equation 8.21

end
L=LHSV_inv(2)/LHSV_inv(1);
kapp_ratio=kapp_rhob(1)/kapp_rhob(2);
n=log10(kapp_ratio)/log10(L);

//CALCULATION (Ex8.3.b)
//FOR SULPHUR
D_CHS=(7.4*(10^(-8))*(Chi*M_B)^(0.5)*T_K)/(myu*(V_A)^0.6);
D_e_S=Epsilon_by_tau*D_pore_by_D_bulk*D_CHS;
epsilon_holdup=0.6;// Assuming bed consists 60% catalyst
k_app_S=k_app_rhob/(3600*epsilon_holdup);//Refer Ex8.3.a
phi_app_S=R*(k_app_S/D_e_S)^(0.5);
//FOR H2
C_H2_corrected=C_H2_incorrect*(P_correct/P_incorrect);
C_S_initial=m_feed*percent_S*10^(-2)/MW_S;
```

```
Initial_rate=k_app_rhob*C_S_initial;
k_app_H2=N_H2*Initial_rate/(3600*epsilon_holdup*C_H2_corrected);
//Assume D_H2 is three times the value given by the Wilke Chang Equation
D_H2=3*(7.4*(10^(-8))*(Chi*M_B)^(0.5)*T_K)/(myu*(V_H2)^0.6);
D_e_H2=Epsilon_by_tau*D_H2;
phi_app_H2=R*(k_app_H2/D_e_H2)^(0.5);

//OUTPUT (Ex8.3.a)
mprintf('\n OUTPUT Ex8.3.a');
mprintf('\n=========================================================================================');
mprintf('\n\tThe Apparent rate constants are \n\t Run1 %0.2f hr-1 \n\t Run2 %0.2f hr-1 ',kapp_rhob(1),kapp_rhob(2))
mprintf('\n\tThe exponent value = %0.1f hence the difference is not consistent with repect to equations (8.23) and (8.24) for the apparent rate constants obtained',n);
mprintf('\n\tThe error may be due to error in assuming a first order reaction');

//OUTPUT (Ex8.3.b)
mprintf('\n\n\n OUTPUT Ex8.3.b');
mprintf('\n=========================================================================================');
mprintf('\n\tThe internal effectiveness factor based on Sulphur and Hydrogen diffusion are %0.2f and %0.2f respectively',phi_app_S,phi_app_H2);
mprintf('\n\tThe internal effectiveness factor based on Hydrogen is negligible');

//FILE OUTPUT
fid= mopen('.\Chapter8-Ex3-Output.txt','w');
```

```
mfprintf(fid,'\n OUTPUT Ex8.3.a');
mfprintf(fid,'\n ========================================================================');
mfprintf(fid,'\n\tThe Apparent rate constants are \n\t Run1 %0.2f hr-1 \n\t Run2 %0.2f hr-1  ',kapp_rhob(1),kapp_rhob(2))
mfprintf(fid,'\n\tThe exponent value = %0.1f hence the difference is not consistent with repect to equations (8.23) and (8.24)for the  apparent rate constants obtained',n);
mfprintf(fid,'\n\tThe error may be due to error in assuming a first order reaction');
mfprintf(fid,'\n\n\n OUTPUT Ex8.3.b');
mfprintf(fid,'\n ========================================================================');
mfprintf(fid,'\n\tThe internal effectiveness factor based on Sulphur and Hydrogen diffusion are %0.2f and %0.2f respectively',phi_app_S,phi_app_H2);
mfprintf(fid,'\n\tThe internal effectiveness factor based on Hydrogen is negligible');
mclose(fid);
//=====================================================END OF PROGRAM================================================
```

# Chapter 9

# Fluidized Bed Reactors

**Scilab code Exa 9.1** `Model II Volumetric Mass Transfer Coefficient K`

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc.,USA,pp 436.
//Chapter-9 Ex9.1 Pg No.376
//Title:Model II- Volumetric Mass Transfer Coefficient (K)
//==========================================================================================================

clear
clc
//INPUT
u0=[ 0.1 0.3 0.5 0.75 0.95 1.15];//Fluid Velocities (m/sec)
X=[0.923 0.872 0.846 0.775 0.728 0.664];//Conversion
h_by_h0=[1.26 1.44 1.66 2.0 2.3 2.7];//Height of bed under fluidized condition by height of packed bed
Epsilon_m=0.456;//Fraction of voids in packed bed
```

```
h0=0.75;//Height of packed bed (m)
k_r=4.45 ;//Reaction rate constant(sec-1)
W=5;//Weight of the bed (kg)


//CALCULATION
n=length(X);
for i=1:n
    K0_L_by_u0(i)=log(1/(1-X(i)));//Refer equation 9.21 Pg No.371
    L(i)=h_by_h0(i)*h0;
    one_minus_epsilon(i)=(1-Epsilon_m)/h_by_h0(i);
    k_rhob(i)=k_r*one_minus_epsilon(i);
    K0(i)=K0_L_by_u0(i)*u0(i)/L(i);
    K(i)=1/((K0(i).^(-1))-(1/k_rhob(i))); //Refer equation 9.19 Pg No.371
end


//OUTPUT
mprintf('\nThe values of K for given velocities')
mprintf('\n u (m/sec) \t K (sec-1) ');
mprintf('\n====================================================================================================');
for i=1:n
    mprintf('\n %.3g \t \t %0.3f',u0(i),K(i));
end

//FILE OUTPUT
fid= mopen('.\Chapter9-Ex1-Output.txt','w');
mfprintf(fid,'\nThe values of K for given velocities')
mfprintf(fid,'\n u (m/sec) \t K (sec-1) ');
mfprintf(fid,'\n====================================================================================================');
for i=1:n
```

```
    mfprintf(fid,'\n %.3g \t \t %0.3f',u0(i),K(i));
end

//==================================================================END OF PROGRAM==================================================================
```

**Scilab code Exa 9.2** `Model II Fraction unconverted naphthalene`

```
//Harriot P.,2003,Chemical Reactor Design (I-Edition) Marcel Dekker,Inc.,USA,pp 436.
//Chapter-9 Ex9.2 Pg No.389
//Title: Model II-Fraction unconverted naphthalene
//==============================================================================================================

clear
clc
//INPUT
D=2.13 ;//Reactor Diameter(m)
L=7.9;//Reactor length (m)
dp_bar= 53*10^(-6);//Particle size (m)
u_mf=0.077;//Minimum fluidzation velocity(cm/s)
u_mb=0.5;//Minimum bubbling velocity(cm/s)
rho_bulk=770;//Bulk density (kg/m3)
rho_b=350;//Density (kg/m3)
Epsilon_m=0.44;//Porosity of bed
T_K=636;//Reaction Temperature (K)
P=266;//Reaction Pressure (kPa)
k_1=1.8;//Reaction rate constant (sec-1)
k_2=k_1;
u0=0.43;//Velocity (m/sec)
C0=2*10^(-2);//Initial concentration (%)
```

```

//CALCULATION
k=k_1+k_2;
one_minus_epsilon=(1-Epsilon_m)*(rho_b/rho_bulk);
k_corrected=k*one_minus_epsilon;//based on bed volume
Nr=k_corrected*L/u0;
K=0.8;//From figure 9.12 at u0=0.43m/sec Pg No.376
Nm=K*L/u0;//Refer equation 9.21 Pg No.371
N=1/((1/Nm)+(1/Nr));//Refer equation 9.22 Pg No.371
X=(1-exp(-N));//Refer equation 9.23 Pg No.371
C_out=(1-X)*C0;
C_out_ppm=C_out*(10^6);

//OUTPUT
mprintf('\nThe fraction of naphthalene unconverted is %0.0f ppm ',C_out_ppm);

//FILE OUTPUT
fid= mopen('.\Chapter9-Ex2-Output.txt','w');
mfprintf(fid,'\nThe fraction of naphthalene unconverted is %0.0f ppm ',C_out_ppm);
mclose(fid);


//==========================================================END OF PROGRAM ===================================================================
```

# Chapter 10

# Novel Reactors

**Scilab code Exa 10.1** `Fraction unconverted naphthalene based on model II`

```
//Harriot P., 2003, Chemical Reactor Design (I-Edition), Marcel Dekker, Inc., USA, pp 436.
//Chapter-10 Ex10.1 Pg No. 408
//Title:Fraction unconverted naphthalene based on model II
//==========================================================================
clear
clc
//INPUT
T_ref=273;//Reference Temperature
T_feed=300+T_ref;//Temperature in (K)
SV_STP=[60000 120000];//Space velocity(Hr-1)
t_cell=0.04;//Thickness(cm)
cell_unit_area=100/(2.54^2);//No of cells per unit area(cells/cm2)
L_inch=6;// Length of monolithic converter (Inches)
Epsilon=0.68;//Porosity
```

```
myu=0.0284*(10^-2);//Viscosity of air(Poise)
rho=6.17*10^(-4);//Density of air (g/cm3)


//CALCULATION
d=sqrt(1/cell_unit_area)- t_cell;
Epsilon=(d^2/(d+t_cell)^2);

//Assume the wash coating lowers d to 0.21 cm and Epsilon to 0.68:
d_new=0.21;
Epsilon_new =0.68
a=4*Epsilon_new/d_new;
SV=SV_STP.*(T_feed/(T_ref*3600));//Refer equation 10.13
L_cm=L_inch*2.54;
u0=SV.*(L_cm);
u=u0.*(1/Epsilon);
Nu=myu/rho;//Kinematic viscosity
D_CO_N2_1=0.192;//Diffusion coefficients for binary gas mixtures(cm2/sec) at 288K
D_CO_N2_2=D_CO_N2_1*(T_feed/288)^(1.7);////Diffusion coefficients for binary gas mixtures(cm2/sec) at 573K
Sc=Nu/D_CO_N2_2;
for i=1:2
Re(i)=d_new*u(i)/Nu;
Re_Sc_d_by_L(i)=Re(i)*Sc*(d_new/L_cm);
Sh(i) = 3.66 *(1+0.095*Re_Sc_d_by_L(i))^(0.45);//Refer equation 10.7
k_c(i)=Sh(i)*D_CO_N2_2/d_new;
X(i)=1-exp((-k_c(i)*a*L_cm*u0(i)^(-1)));//Refer equation10.12
Percent_X(i)=X(i)*100;
end

//OUTPUT
mprintf('\n The Conversion expected for the given
space velocities ');
mprintf(' \n Space Velocity (hr-1)\t \t Conversion (%%)');
mprintf('\n ==================================================================================== ');
for i=1:2
    mprintf('\n %.0f \t \t \t \t %.1f',SV_STP(i),Percent_X(i));
end

//FILE OUTPUT
fid= mopen('.\Chapter10-Ex1-Output.txt','w');
mfprintf(fid,'\n The Conversion expected for the given space velocities ');
mfprintf(fid,' \n Space Velocity (hr-1)\t \t Conversion (%%)');
mfprintf(fid,'\n ==================================================================================== ');
for i=1:2
    mfprintf(fid,'\n %.0f \t \t \t \t %.1f',SV_STP(i),Percent_X(i));
end
mclose(fid);


//============================================================================ END OF PROGRAM ===============================================================================
```

**Scilab code Exa 10.2** Conversion as a function of No of Gauzes

```
//Harriot P., 2003, Chemical Reactor Design (I-Edition), Marcel Dekker, Inc., USA, pp 436.
//Chapter-10 Ex10.2 Pg No. 414
//Title:Conversion as a function of No. of Gauzes
//
clear
clc
// COMMON INPUT
M_NH3=17;//Molecular weight NH3
M_air=29;//Molecular weight air
f_air=0.9;//Fraction of air in feed
f_NH3=(1-f_air);//Fraction of NH3 in feed
myu_air=0.0435*(10^-2);//Viscosity of air (Poise)
P_atm=(100+14.7)/14.7;//Pressure of the system
P_ref=1;//Reference Pressure
T_ref=273;//Reference temperature
T_inlet=300+T_ref;//Inlet Temperature
V_ref=22400;
T_surf=700+T_ref;//Surface Temperature
u0=1.8;//Velocity at 300 C (m/sec)
d=0.076*(10^-1);//Size of wire (cm)
D_NH3_N2=0.23;//Diffusivity at 298 K 1 atm(cm2/s)
N=32;//Gauzes (wires/cm)
frac_N2 = 0.25*(10^(-2));//Fraction of NH3 fed into N2 (Byproduct reaction)
n =[1 2 5 10 15 20];//No. of Gauzes


//CALCULATION (Ex 10.2.a)
M_ave =f_air*M_air+f_NH3*M_NH3;
rho =(M_ave*T_ref*P_atm)/(V_ref*T_surf*P_ref);
u0_surf = u0*(T_surf/T_inlet);
Re = rho*u0_surf*100*d/myu_air;
Gamma = [1-32*(d)]^2;//From equation 10.5
Re_Gamma = Re/Gamma;
D_NH3 = 0.23*(T_surf/298)^(1.7)*(1/7.8);// at 7.8
```

```
   atm 700  C
Sc =(myu_air*P_ref)/(rho*D_NH3);
j_D = 0.644*(Re_Gamma)^(-0.57);//Refer equation
   10.14
k_c = j_D*(u0_surf*100/Gamma)*(1/(Sc)^(2/3));
a_dash = 2*(%pi)*(d)*N
k_c_a_dash_u0 =(k_c*a_dash)/(u0_surf*100);
m = length(n)
for i = 1:m
    X(i) = (1-exp(-k_c_a_dash_u0*n(i)));
end
//CALCULATION (Ex 10.2.b)
for i = 1:m
    X(i) = (1-exp(-k_c_a_dash_u0*n(i)));
    Yield(i) = X(i)-frac_N2*n(i);
end


//OUTPUT(Ex 10.2.a)
mprintf('\n OUTPUT Ex10.2.a');
mprintf('\n=====================================================');
mprintf('\n \tThe Ammonia Conversion');
mprintf('\n=====================================================');
mprintf('\n\t Gauzes          Conversion');
mprintf('\n\t  (n)               (X)');
mprintf('\n=====================================================');
for i=1:m
    mprintf('\n\t  %.0f  \t \t %.3f',n(i),X(i));
end

//OUTPUT(Ex 10.2.b)
mprintf('\n\n\n OUTPUT Ex10.2.b');
mprintf('\n
   =====================================================');
mprintf('\n \tThe Ammonia Yield');
mprintf('\n
   =====================================================');
mprintf('\n\t Gauzes          Yield');
mprintf('\n\t  (n)               (X-%fn)',frac_N2);
mprintf('\n ============================================');
for i=1:m
    mprintf('\n\t  %.0f \t \t %.3f',n(i),Yield(i));
end
//FILE OUTPUT
fid= mopen('.\Chapter10-Ex2-Output.txt','w');
mfprintf(fid,'\n OUTPUT Ex10.2.a');
mfprintf(fid,'\n =======================================');
mfprintf(fid,'\n \tThe Ammonia Conversion');
mfprintf(fid,'\n =======================================');
mfprintf(fid,'\n\t Gauzes          Conversion');
mfprintf(fid,'\n\t  (n)               (X)');
mfprintf(fid,'\n =======================================');
for i=1:m
    mfprintf(fid,'\n\t  %.0f  \t \t %.3f',n(i),X(i));
end
mfprintf(fid,'\n\n\n OUTPUT Ex10.2.b');
mfprintf(fid,'\n ============================================');
mfprintf(fid,'\n \tThe Ammonia Yield');
mfprintf(fid,'\n ============================================');
mfprintf(fid,'\n\t Gauzes          Yield');
mfprintf(fid,'\n\t  (n)               (X-%fn)',frac_N2);
mfprintf(fid,'\n ============================================');
for i=1:m
    mfprintf(fid,'\n\t  %.0f \t \t %.3f',n(i),Yield(i));
end
mclose(fid);
```

```

//
    END OF PROGRAM
```