<u>**CL312**</u>

Lab Report 5

Name: Shalin Jain, Shree Kumar Sundaray, Shridam Mahajan, Shubham Kumar Gupta, Shubham Raj

Roll No.: 180107055, 180107056, 180107057, 180107058, 180107059

Group: 11

The irreversible vapor-phase cracking reaction of acetone (A) to ketene (B) and methane (C) is carried out adiabatically in a plug-flow reactor. The reaction is first order with respect to acetone and the reaction rate is given by $-r_A = kC_A$ (C_A: concentration of acetone, gmol/m^3). From the mass balance equations for the plug-flow reactor, the rate of change of the molar flow rate of each species F_A, F_B, and F_C (gmol/sec) with respect to reactor volume V is given by

$$\frac{dF_A}{dV} = r_A \;,\; \frac{dF_B}{dV} = -r_A \;,\; \frac{dF_C}{dV} = -r_A$$

The rate constant k (sec^{-1}) can be expressed as a function of temperature T (K):

$\ln k = 34.34\text{-}34222/T$

For a gas-phase reactor, the concentration of the acetone C_A (gmol/m^3) can

be represented as C_A =- $1000 y_A P/8.31T$

The mole fraction of species i, y_i, is given by
$y_i = F_i/F_A+F_B+F_C$ (i=A,B,C),

and the conversion of acetone can be calculated from $X_A = F_{A0}-F_A/F_{A0}$

An energy balance on a differential volume of the reactor yields

$$\frac{dT}{dV} = \frac{-r_A(-\Delta H)}{F_A C_{pA} + F_B C_{pB} + F_C C_{pC}}$$

where ΔH (J/gmol) is the heat of reaction at temperature T and C_{pi}(i = A, B, C) are the molar heat capacities (J/(gmol·K)) of acetone (A), ketene (B), and methane (C) and are given by

$$\Delta H = 80{,}700 + 6.8(T - 298) - 0.00575(T^2 - 298^2) - 1.27 \times 10^{-6}(T^3 - 298^3)$$

$$C_{pA} = 26.2 + 0.183T - 45.86 \times 10^{-6}T^2,\ C_{pB} = 20.04 + 0.0945T - 30.95 \times 10^{-6}T^2$$

$$C_{pC} = 13.39 + 0.077T - 18.91 \times 10^{-6}T^2$$

The acetone feed flow rate to the reactor is 8000 kg/hr (=38.3 gmol/sec), the inlet temperature is T = 1150 K, and the reactor operates at the constant pressure of P = 162 kPa (1.6 atm). The volume of the reactor is $4m^3$.

1. Calculate the flow rate (gmol/sec) and the mole fraction of each species at the reactor outlet.
2. In order to increase the conversion of acetone, it is suggested to feed nitrogen along with the acetone. The total molar feed rate is maintained constant as 38.3 gmol/sec. Calculate the final conversions and temperatures for the case where 28.3, 18.3, 8.3, 3.3, and 0.0 gmol/sec nitrogen is fed into the reactor and plot the results as a function of reactor volume. The heat capacity of nitrogen is given by:

$$C_{pN2} = 6.25 + 0.00878T - 2.1 \times 10^{-8}T^2$$

3. Calculate the final conversions and temperatures in the reactor operating at a pressure range of 1.6 atm≤P≤5 atm for acetone feed rates of 10, 20, 30, 35, and 38.3 gmol/ sec. The inlet temperature is T=1035 K and nitrogen is fed to maintain the total feed rate 38.3 gmol/sec in all cases. Prepare plots of final conversion versus P and F_{A0} and final temperature versus P and F_{A0}

Solution 1:-

Algorithm:-

- First we write a matlab script ode_solver.m for the system of differential equations.
- The input arguments are V, X and pf; where V denotes volume from 0 to reactor volume = 4 m^3; X is an array of size 4 with X(1) = F_A, X(2) = F_B, X(3) = F_C flow rates, and X(4) = T, temperature.; pf is an array of size 2 with pf(1) = P, pressure, and pf(2) = FN2, Nitrogen flow rate. The function returns matrix X with 4 columns.
- Then in a different script we initialize the parameters pf, Vspan (reactor volume) and initial vector X0.
- Then we solve the differential equations using built in ode45 method calling ode_solver as its argument.
- Then we calculate F_A, F_B, F_C and T by taking the 1^{st}, 2^{nd}, 3^{rd} and 4^{th} elements of last row of the matrix X respectively.

Code:-

Matlab script for differential equations:

```
function dX = ode_solver(V,X,pf)
%differential equations for cracking of acetone
P = pf(1);
FN2 = pf(2);
T = X(4);
CA = 1000*(X(1)./(X(1)+X(2)+X(3)+FN2))*P/(8.31*T);
k = exp(34.34-34222/T);
dH = 80770+6.8*(T-298)-(5.75e-3)*(T^2 - 298^2)-(1.27e-6)*(T^3 -
298^3);
CpA = 26.2 + 0.183*T - (45.86e-6)*T^2;
CpB = 20.04 + 0.0945*T - (30.95e-6)*T^2;
```

```
  CpC = 13.39 + 0.077*T - (18.91e-6)*T^2;
  CpN2 = 6.25 + 0.00878*T - (2.1e-8)*T^2;
  rA = -k.*CA;
  %using dFA/dV,dFB/dV,dFC/dV and dT/dV.
  dX = [rA; -rA; -rA; -rA*(-dH./(X(1)*CpA + X(2)*CpB + X(3)*CpC +
FN2*CpN2))];
end
```

Matlab script for solving 1:

```
clc
pf = [162 0]; %Pressure in kPa and feed nitrogen in gmole/sec
Vspan = [0 4]; %volume of reactor covered at inlet and outlet
X0 = [38.3 0 0 1150]; %initial values of molar flow rate of A,B,C
and temperature respectively
[V X] = ode45(@ode_solver, Vspan, X0, [], pf); %solving using
ode45 method
FA = X(end,1),FB = X(end,2),FC = X(end,3),T = X(end,4)
```

Solution 2:-

Algorithm:-

- First we write a matlab script ode_solver.m for the system of differential equations.
- The input arguments are V, X and pf; where V denotes volume from 0 to reactor volume = 4 m^3; X is an array of size 4 with X(1) = F_A, X(2) = F_B, X(3) = F_C flow rates, and X(4) = T, temperature.; pf is an array of size 2 with pf(1) = P, pressure, and pf(2) = FN2, Nitrogen flow rate. The function returns matrix X with 4 columns.
- Then in a different script we initialize the parameters P(pressure), Vspan (reactor volume) and vector FN2(initial flow rates of Nitrogen).
- Then we run a loop through all the elements of FN2.
- We initialize the parameters for ode_solver X0 with F_A=38.3-FN2(idx) where idx is the index of loop, F_B=0, F_C=0 and T=1150 K, and pf with pf(1) = P and pf(2) = FN2(idx), where idx is the index of the loop.
- Then we solve the differential equations using built in ode45 method calling ode_solver as its argument.
- Then we find conversion xfc(idx) and temperature Tr(idx), where idx is the index of the loop.
- We plot the graphs for xc vs V and Tr vs V.

Code:-

Matlab script for differential equations:

```
  function dX = ode_solver(V,X,pf)
  %differential equations for cracking of acetone
  P = pf(1);
  FN2 = pf(2);
  T = X(4);
  CA = 1000*(X(1)./(X(1)+X(2)+X(3)+FN2))*P/(8.31*T);
  k = exp(34.34-34222/T);
  dH = 80770+6.8*(T-298)-(5.75e-3)*(T^2 - 298^2)-(1.27e-6)*(T^3 -
298^3);
  CpA = 26.2 + 0.183*T - (45.86e-6)*T^2;
  CpB = 20.04 + 0.0945*T - (30.95e-6)*T^2;
  CpC = 13.39 + 0.077*T - (18.91e-6)*T^2;
  CpN2 = 6.25 + 0.00878*T - (2.1e-8)*T^2;
  rA = -k.*CA;
  %using dFA/dV,dFB/dV,dFC/dV and dT/dV.
  dX = [rA; -rA; -rA; -rA*(-dH./(X(1)*CpA + X(2)*CpB + X(3)*CpC +
FN2*CpN2))];
end
```

Matlab script for solving part 2:

```
clc
clear all
P = 162; %Pressure in kPa and feed nitrogen in gmole/sec
Vspan = [0 4]; %volume of reactor covered at inlet and outlet
FN2 = [28.3 18.3 8.3 3.3 0.0]; nF = length(FN2);  %flow rates of
Nitogen
for i = 1:nF
    X0 = [38.3-FN2(i) 0 0 1150];%initial X with varying N2 flow
rates.
    pf = [P FN2(i)]; %initialzing pf
    [V X] = ode45(@ode_solver, Vspan, X0, [], pf); %solving using
ode45 method
    figure(1) %plotting T vs V.
    plot(V,X(:,4)), xlabel('Reactor volume(m^3)'),
ylabel('Temperature(K)'),
    legend('FN2 = 28.3','FN2 = 18.3','FN2 = 8.3','FN2 = 3.3','FN2
= 0.0');
```

```
    hold on;
end
for i = 1:nF
    X0 = [38.3-FN2(i) 0 0 1150];
    pf = [P FN2(i)];
    [V X] = ode45(@ode_solver, Vspan, X0, [], pf);
    xc = (X0(1) - X(:,1))/X0(1); Tr(i) = X(end,4); %finding x and
T
    xfc(i) = (X0(1) - X(end,1))/X0(1);
    figure(2) %plotting conversion vs Volume
    plot(V,xc), xlabel('Reactor volume(m^3)'),
ylabel('Conversion');
    legend('FN2 = 28.3','FN2 = 18.3','FN2 = 8.3','FN2 = 3.3','FN2
= 0.0');
    hold on;
end
fprintf('final conversion array'); xfc
fprintf('\nTemperature array'); Tr
```

Solution 3:-

Algorithm:-

- First we write a matlab script ode_solver.m for the system of differential equations.
- The input arguments are V, X and pf; where V denotes volume from 0 to reactor volume = 4 m^3; X is an array of size 4 with X(1) = F_A, X(2) = F_B, X(3) = F_C flow rates, and X(4) = T, temperature.; pf is an array of size 2 with pf(1) = P, pressure, and pf(2) = FN2, Nitrogen flow rate. The function returns matrix X with 4 columns.
- Then in a different script we initialize the parameters P vector (pressure range) with length nP, Vspan (reactor volume) and vector FA0(flow rates of acetone) with length nF, FN2 vector(nitrogen flow rates) as 38.3-FA0.
- We initialize concentration xc and temperature T matrix of size nFXnP.
- Then we run a double loop through all the elements of xc and T
- We initialize the parameters for ode_solver X0 with F_A=FA0(idx1) where idx1 is the index of outer loop, F_B=0, F_C=0 and T=1035 K, and pf with pf(1) = P(idx2) and pf(2) = FN2(idx1), where idx2 is the index of inner loop, and idx1of outer loop.
- Then we solve the differential equations using built in ode45 method calling ode_solver as its argument.
- Then we update xc(idx1,idx2) and temperature T(idx1,idx2) of the matrix, where idx1 is the index of outer loop and idx2 of inner loop.
- We plot the graphs for X_A vs P and T vs P for different acetone flow rates $F_{A0.}$

Code:-

Matlab script for differential equations:

```
function dX = ode_solver(V,X,pf)
  %differential equations for cracking of acetone
  P = pf(1);
  FN2 = pf(2);
  T = X(4);
  CA = 1000*(X(1)./(X(1)+X(2)+X(3)+FN2))*P/(8.31*T);
  k = exp(34.34-34222/T);
  dH = 80770+6.8*(T-298)-(5.75e-3)*(T^2 - 298^2)-(1.27e-6)*(T^3 -
298^3);
  CpA = 26.2 + 0.183*T - (45.86e-6)*T^2;
  CpB = 20.04 + 0.0945*T - (30.95e-6)*T^2;
  CpC = 13.39 + 0.077*T - (18.91e-6)*T^2;
  CpN2 = 6.25 + 0.00878*T - (2.1e-8)*T^2;
  rA = -k.*CA;
  %using dFA/dV,dFB/dV,dFC/dV and dT/dV.
  dX = [rA; -rA; -rA; -rA*(-dH./(X(1)*CpA + X(2)*CpB + X(3)*CpC +
FN2*CpN2))];
end
```

Matlab script for solving part 3:

```
P = [1.6:0.2:5]*101.325; %initializing pressure range
Vspan = [0 4]; %initailzing reactor volume
FA0 = [10 20 30 35 38.3]; %initialzing acetone flow rates
FN2 = 38.3-FA0; nP = length(P); nF = length(FA0);
xc = zeros(nF,nP); T = zeros(nF,nP); %initialzing concentartion
and temperature matrix
for i = 1:nF
    for j = 1:nP
        X0 = [FA0(i) 0 0 1035]; pF = [P(j) FN2(i)]; %initialzing
parameters X and pf
        [V X] = ode45(@ode_solver, Vspan, X0, [], pF);%solving
using ode45 method
        xc(i,j) = (X0(1)-X(end,1))/X0(1);
        T(i,j) = X(end,4);
    end
```

```
end
P = P/101.325;
%plotting T vs P
figure(3)
plot(P,T(1,:),'o',P,T(2,:),'*',P,T(3,:),'x',P,T(4,:),'d',P,T(5,:)
,'v')
xlabel('P(atm)'), ylabel('T(K)'),grid
legend('F_A0 = 10','F_A0 = 20','F_A0 = 30','F_A0 = 35','F_A0 =
38.3');
%plotting XA vs P.
figure(4)
plot(P,xc(1,:),'o',P,xc(2,:),'*',P,xc(3,:),'x',P,xc(4,:),'d',P,xc
(5,:),'v')
xlabel('P(atm)'), ylabel('x_A'),grid
legend('F_A0 = 10','F_A0 = 20','F_A0 = 30','F_A0 = 35','F_A0 =
38.3');
```

Results:-

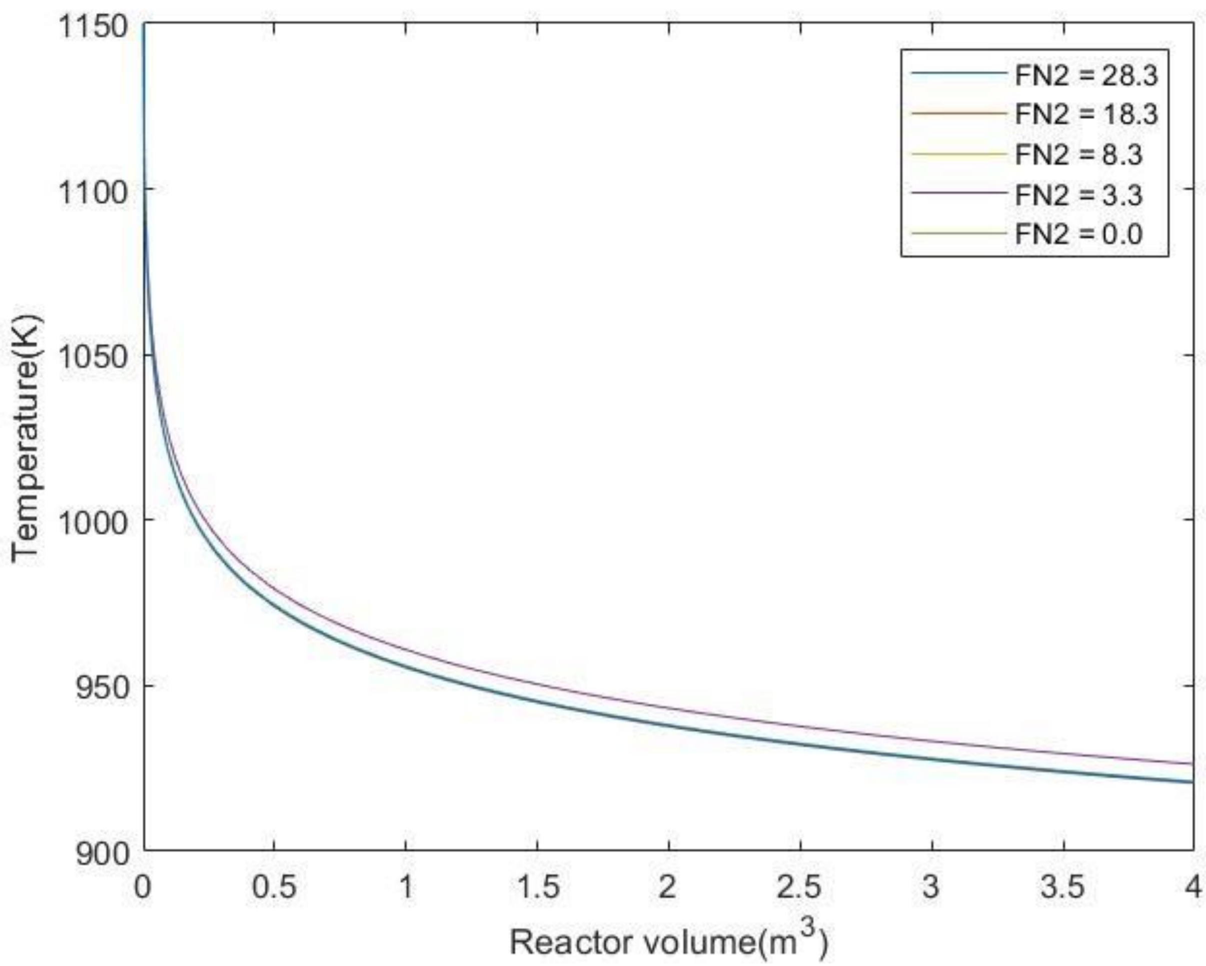
Part 1:-

FA = 19.9777gmol/sec, F B =18.3223gmol/sec, FC =18.3223gmol/sec and T = 920.8778K

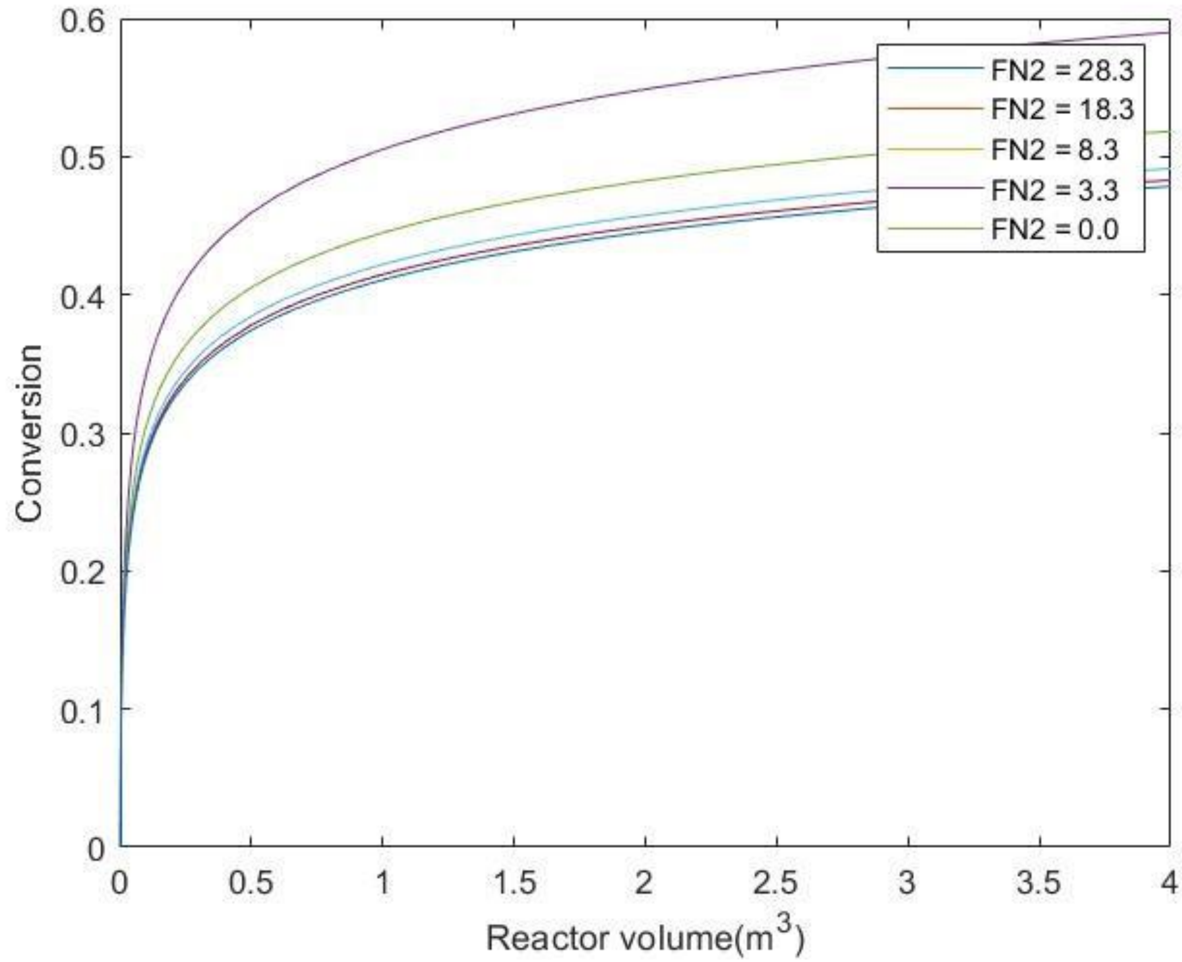
Part 2:-

Nitrogen rate (gmol/sec)	28.3	18.3	8.3	3.3	0
Final conversion	0.5899	0.5183	0.4913	0.4829	0.4784
Final temperature (K)	926.3222	921.0767	920.4939	920.6749	920.8778

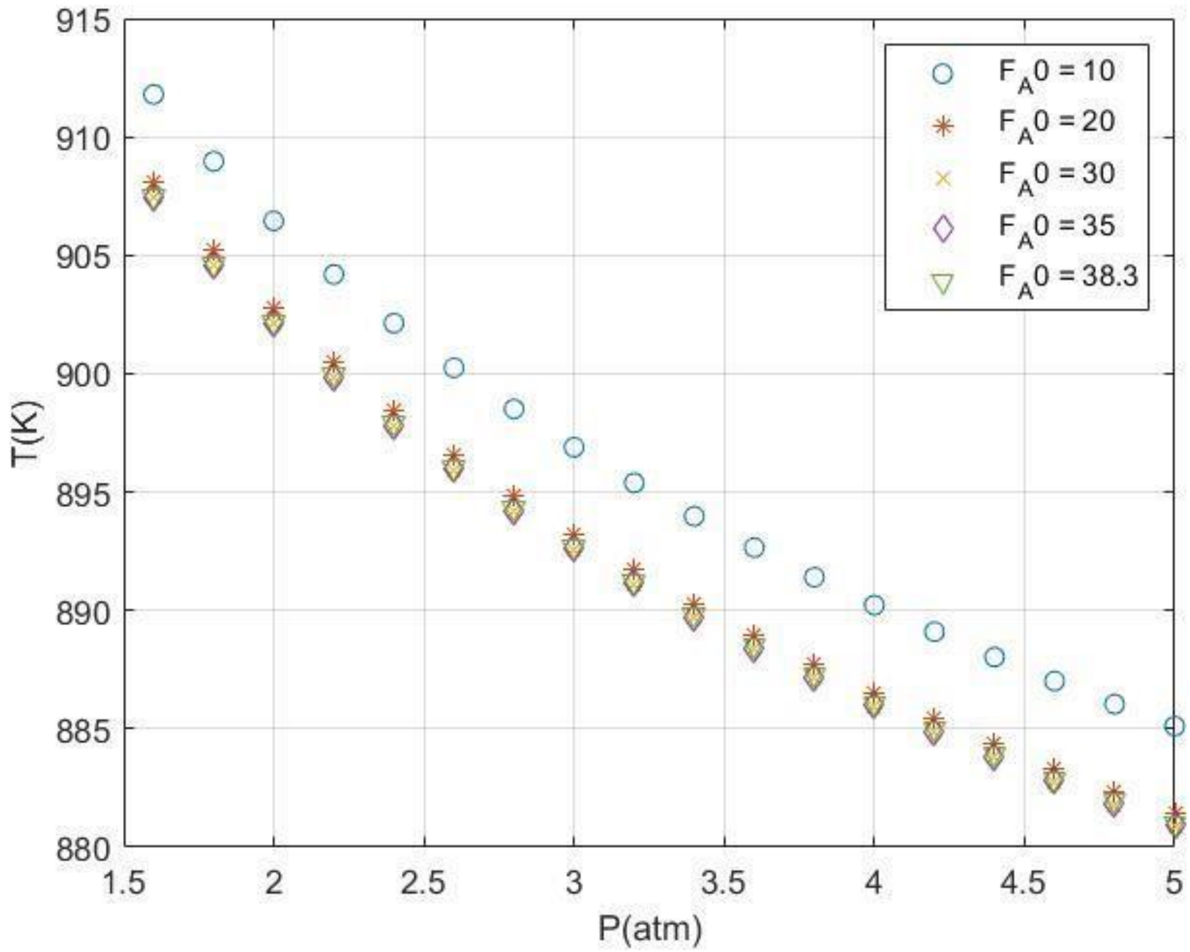
Plots for xc vs V and Tr vs V:-

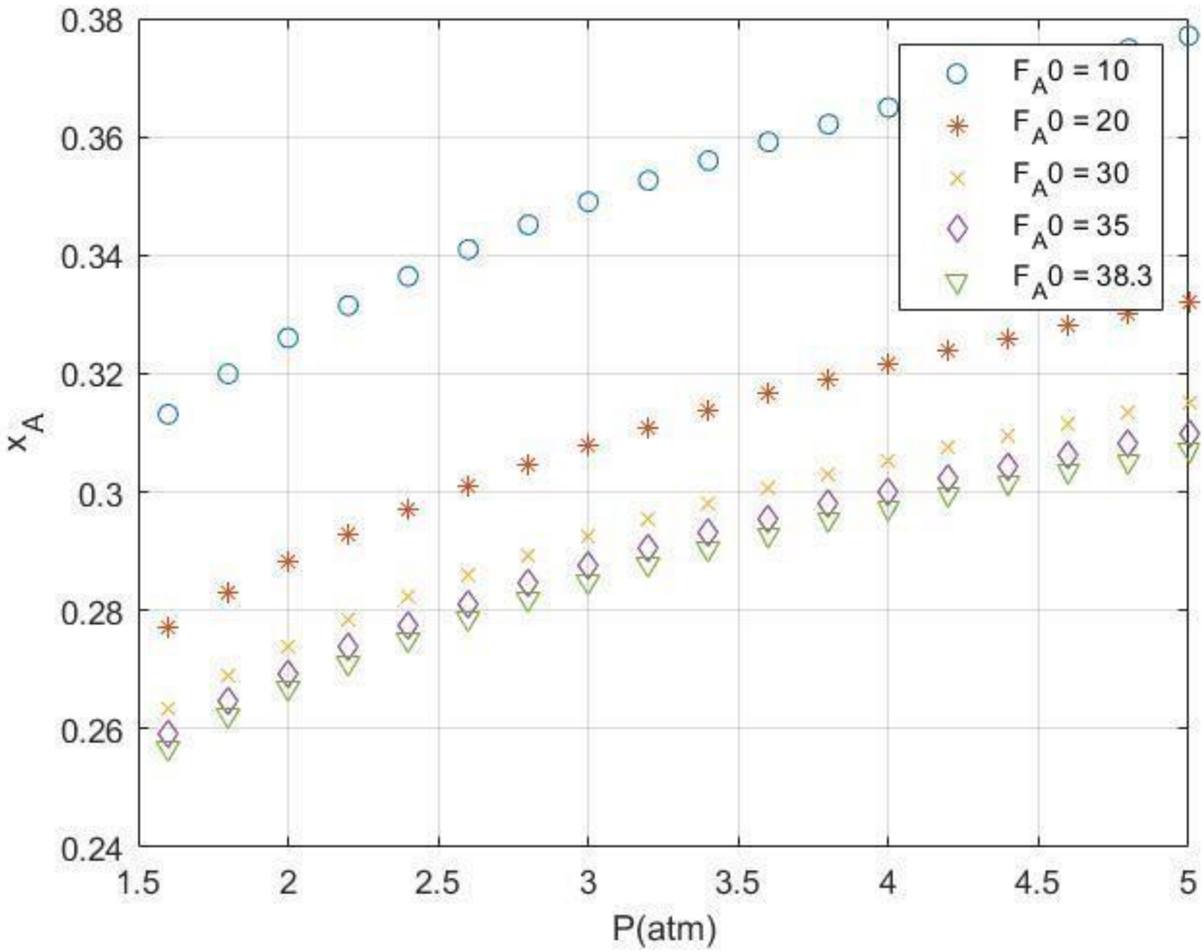


FN2 = 28.3
FN2 = 18.3
FN2 = 8.3
FN2 = 3.3
FN2 = 0.0
Temperature(K)
Reactor volume(m^3)
1150
1100
1050
1000
950
900
0
0.5
1
1.5
2
2.5
3
3.5
4



Part 3:- Plots for X_A vs P and T vs P for different acetone flow rates F_{A0} :-


915
910
905
900
895
890
885
880
T(K)
1.5
2
2.5
3
3.5
4
4.5
5
P(atm)
F_A0 = 10
F_A0 = 20
F_A0 = 30
F_A0 = 35
F_A0 = 38.3



0.38
0.36
0.34
0.32
0.3
0.28
0.26
0.24
1.5
2
2.5
3
3.5
4
4.5
5
P(atm)
x_A
$F_A0 = 10$
$F_A0 = 20$
$F_A0 = 30$
$F_A0 = 35$
$F_A0 = 38.3$