

Dear Students: Please answer all questions

1. Consider an irreversible second-order reaction, $2A \rightarrow B$ (with rate, $-r_A = kCA^2$) that has been carried out in a batch reactor. The initial concentration is 1 mol/litre, and after 30 minutes the concentration is 0.25 mol/litre. What is the value of the second-order rate constant? Show units

Now, the reaction is to be conducted in a plug flow reactor, with a feed concentration of 1 mol/litre and a flowrate of 2 liters/minute. To achieve an outlet concentration of 0.25 mol/liter, what should be the volume of the PFR? (25 Marks)

2. The exothermic reaction $A \rightarrow B + C$

was carried out adiabatically and the following data recorded:

X	0.0	0.2	0.4	0.45	0.5	0.6	0.8	0.9
$-r_A$ (mol/dm ³ .min)	1	1.67	5	5	5	5	1.95	0.91

The entering molar flow rate of A was 300 mol. min⁻¹.

- What are the PFR and CSTR volumes necessary to achieve 40% conversion?
- Over what range of conversions would the CSTR and PFR reactor volumes be identical?
- What is the maximum conversion that can be achieved in a 105 dm³ CSTR? (25Marks)

3. Answer the following questions:

- Define the term 'specific reaction rate' or 'rate of reaction'.
- What are the variables affecting the rate of reaction?
- A large CSTR, small CSTR and PFR of fixed volume are available. In general, how would you arrange them for getting maximum conversion for reactions of order >1 and <1 . Why?
- Calculate the activation energy for the decomposition of benzene-diazonium-chloride to give chlorobenzene and nitrogen, first order reaction, using the following data;

k (Sec ⁻¹)	0.00043	0.00103	0.0018	0.00355	0.00717
T (K)	313	318	323	328	333

Also find the rate equation.

Department: Chemical Engineering
Stage/ Year: Third
Total Mark: 100

Course Title: Reactor design
Course Code: KOU20443
Time Allowed: 90 minutes
Attached Sheet:

(25 Marks)

4. The first order liquid phase reaction $A + B \rightarrow C + D$, is carried out in a two CSTRs connected in series with equal volumes. The first reactor is fed by two independent liquid streams. One stream contains reactant A in water, while the other contains reactant B in water. A feed stream containing A at a concentration of exactly 0.1 mol/L with a volumetric flow of 1.8 L/s enters the first reactor. B enters the first reactor in a second stream at an identical concentration and flowrate to that of A. The temperature in both reactors is maintained at 75 °C and the reaction rate constant is equal to 0.65 s^{-1} . Calculate the conversion of A in the outlet stream from the first reactor when the conversion of the second reactor is equal to 90% and then find the total volume of the system.

(25 Marks)



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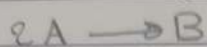
X

X

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X

Q1



$$-r_A = k C_A^2$$

$$C_A = C_{A0} = 1 \frac{\text{mol}}{\text{L}}$$

Batch

$$C_B = C_A = 0.25 \frac{\text{mol}}{\text{L}}$$

$$\frac{1}{25}$$

$$-r_A = k \left[C_A^2 - \frac{1}{K_c} C_B \right]$$

$$K_c = \frac{C_B}{C_A^2}$$

$$-r_A = k \left[1^2 - \frac{1}{0.25} (0.25) \right]$$

$$-r_A = k (0) \left(\frac{\text{mol}}{\text{dm}^3 \cdot \text{s}} \right) = \frac{(0.25)}{1^2}$$

$$-r_A = 0 \frac{\text{mol}}{\text{dm}^3}$$

$$K_c = 0.25$$

PFR

$$C_{A0} = 2$$

$$C_A = 0.25$$

PFR

$$V = \int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A}$$

$$-r_A = k C_A^2$$

$$-r_A = 0.25 (2)^2$$

$$-r_A = 1$$

$$V = \frac{C_A}{C_{A0}} \times \frac{1}{-r_A} =$$

$$V = \frac{0.25}{2} \times \frac{1}{1} = 0.125 \text{ dm}^3$$

$$F_A = v C_A$$

$$C_A = \frac{N_A}{V}$$

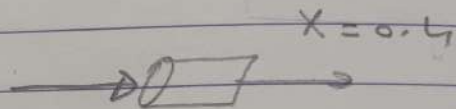
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Q2]



X	0	0.2	0.4	0.25	0.5	0.6	0.8	0.9
-r _A	1	1.67	5	5	5	5	1.95	0.91
F _{A0}	300	179.6	60	60	60	60	153.8	329.7
-r _A								
$\frac{1}{-r_A}$	1	0.6	0.2	0.2	0.2	0.2	0.51	1.1

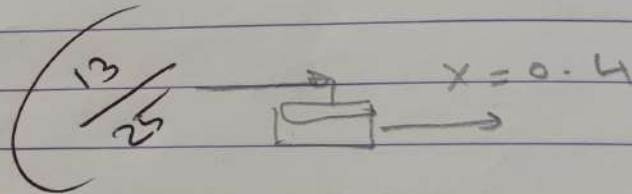
$F_{A0} = 300 \text{ mol/min}$



(a) CSTR

$V = \frac{F_{A0} - F_A}{-r_A} \times X_A$

$V = \frac{60 \times 0.4}{5}$
 $V = 24 \text{ dm}^3$



PFR

$\Delta X = \frac{0.4 - 0}{2} = 0.2$

$V = F_{A0} \int_0^{0.4} \frac{dX}{-r_A}$

$V = \frac{F_{A0}}{F_{A0}} \int_0^{0.4} \frac{dX}{-r_A} = \frac{\Delta X}{3} \left[\frac{F_{A0}}{-r_A(0)} + 4 \frac{F_{A0}}{-r_A(0.2)} + \frac{F_{A0}}{-r_A(0.4)} \right]$

$= \frac{0.2}{3} [300 + 4(179.6) + 60]$

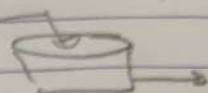
$V = 0.0667 \times 1078.4 = 71.93 \text{ dm}^3$

(b) over 0.6 Because at first one of the reactor can achieve 0.3 conversion after that the other reactor can achieve 0.6 over that range is identical

(c) $V = 105 \text{ dm}^3$

$\max X = ?$

CSTR



$$V = \frac{F_{A0} \cdot X_A}{-r_A}$$

$$F_{A0} \cdot X_A = V \cdot -r_A$$

$$X_A = \frac{105 \cdot 0.59}{300}$$

$\max X_A = 0.207$

$$V = 71.2 \quad -r_A = 0.4$$

$$V = 105 \quad -r_A = ?$$

$$-r_A \cdot 71.2 = 42$$

$$-r_A = 0.59$$

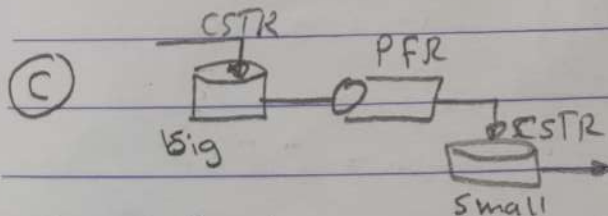
Q3

(a) Specific reaction rate: is a rate of of mole of reactant over the Volume Based on absolute temperature and energy and time

$$k(T) = A e^{-\frac{E}{RT}}$$

$$\frac{20}{25}$$

(b) number of moles, K, activation energy, temperature, volume of reactor and substances (Reactant)



- Because first we need big CSTR to achieve at list 0.3 and leave large Volume for Better capacity the PFR so the kind of the reactor idea achieve 0.3 more then the CSTR (small) cuz we already did the big part reaction. This time we need at list 0.15 more conversion.

d) K	0.00043	0.00103	0.0018	0.00355	0.00717
T(K)	313	318	323	328	333

E = ? $k(T) = A e^{-E/RT}$

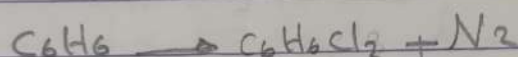
$$\frac{k(T_1)}{k(T_0)} = \frac{A e^{-E/RT_1}}{A e^{-E/RT_0}}$$

$$\ln \left[\frac{k(T_1)}{k(T_0)} \right] = \left[\frac{1}{T_0} - \frac{1}{T_1} \right] E \quad 15$$

$$\ln \left(\frac{0.00043}{0.00717} \right) = \left[\frac{1}{333} - \frac{1}{313} \right] E$$

$$-2.81 = -1.92 \times 10^{-4} E$$

$$E = \frac{-2.81}{-1.92 \times 10^{-4}} = 14635.4 \frac{\text{J}}{\text{mol}} = 14.6354 \frac{\text{kJ}}{\text{mol}}$$



$$-r_A = k C_{\text{C}_6\text{H}_6}$$

Q4



$$T = 75^\circ\text{C}$$

$$k = 0.65 \text{ s}^{-1}$$

$$V_T = ?$$

$$C_{A0} = 0.1 \text{ mol/L}$$

$$v_A = 1.8 \text{ L/s}$$

A
B
C_{B0}

CSTR

X₁ = ?

CSTR

$$X_2 = 0.9$$

$$V_1 = \frac{F_{A0} \cdot X_A}{-r_A}$$

$$V_2 = V_1 = 0.18 \times X_A$$

$$X_1 = \frac{2.49 \times 0.065}{0.18} \rightarrow X_{A1} = 0.899$$

$$V_2 = \frac{F_{A0} \cdot X_{A2}}{-r_A}$$

$$V_2 = 0.18 \times 0.9$$

$$V_2 = 2.49 \text{ dm}^3$$

$$V_T = 2.49 + 2.49 = 4.98 \text{ dm}^3$$

$$-r_A = k C_A$$

$$-r_A = 0.65 \times 0.1$$

$$-r_A = 0.065$$

$$F_{A0} = v C_{A0}$$

$$= 0.1 \times 1.8$$

$$= 0.18$$

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Using the data in the table, calculate the reactor volumes for the CSTR-PFR-CSTR reactors in series sequence along with the corresponding conversion ($X_1=0.4$, $X_2=0.7$, and final conversion is 0.8) with initial molar flowrate 2 mole/dm³.

$$X_1=0.4 \quad X_2=0.7 \quad X_3=0.8$$

X	0	0.2	0.4	0.6	0.8
-r _A	0.010	0.0091	0.008	0.005	0.002

$$\frac{F_{A0}}{-r_A} \rightarrow \begin{matrix} 0 & 22 & 50 & 120 & 400 \end{matrix}$$

CSTR ①

$$V_1 = \frac{F_{A0}}{-r_A} X_1$$

$$= \frac{2}{0.01} \times (0.2)$$

$$V_1 = 40 \text{ dm}^3$$

$$F_{A0} = 2 \text{ mol/dm}^3 \cdot s$$



$$\frac{1}{6}$$

PFR ②

$$V_2 = F_{A0} \int_{X_1}^{X_2} \frac{dX}{-r_A}$$

$$\Delta X = \frac{X_2 - X_1}{2} = \frac{0.7 - 0.4}{2}$$

$$\Delta X = 0.15$$

$$V_2 = \frac{\Delta X}{3} \left[\frac{F_{A0}}{-r_A(X=0.4)} + 4 \frac{F_{A0}}{-r_A(X=0.6)} + \frac{F_{A0}}{-r_A(X=0.7)} \right]$$

$$V_2 = \frac{0.15}{3} \times (50 + (4 \times 120) + (214))$$

$$V_2 = 0.05 \times 744$$

$$V_2 = 37.2 \text{ dm}^3$$

$$\frac{F_{A0}}{-r_A} \bigg|_S$$

$$\frac{0.75}{3.5 \times 10^{-3}}$$

$$X_S = 214.29$$

$$X_S = \frac{0.7 + 0.8}{2}$$

$$X_S = 0.75$$

$$-r_S = 0.005 + 0.002$$

CSTR 2

$$V_3 = \frac{F_{A0}}{-r_{A3}} (X_3 - X_2)$$

$$= \frac{2}{0.008} (0.8 - 0.7)$$

$$V_3 = 25 \text{ dm}^3 \quad \alpha$$

$$V_{\text{overall}} = V_1 + V_2 + V_3$$

$$= 40 + 37.2 + 25$$

$$V = 102.2 \text{ dm}^3$$

Department: Chemical Engineering

Stage/ Year: Third

Total Mark: 100

Course Title: Reactor Design

Course Code: KOU20443

Time Allowed: 120 minutes

Attached Sheet:

Answer All Questions

1. A reaction is to be carried out at 380 K in a PFR. The reaction:



follows an elementary rate law at the reactor operating temperature where the rate constant (k) is 0.62 min^{-1} .

The reactant concentration in the feed stream is 2.22 mol.dm^{-3} and the stream volumetric rate is $6.2 \text{ dm}^3 \text{ min}^{-1}$. For a conversion of 77% what is the:

- (a) Residence time.
(b) Reactor volume required.

(5)

(20 Marks)

2. The elementary, second order, liquid phase reaction $A+B \rightarrow C+D$ is conducted in an isothermal plug flow reactor of 1 m^3 volume. The inlet volumetric flow rate is $10 \text{ m}^3/\text{hr}$ and $CA_0 = CB_0 = 2 \text{ kmol/m}^3$. At these conditions, conversion of A is 50%. Now, if stirred tank reactor of 2 m^3 volume is installed in series, upstream of the plug flow reactor, then what conversion can be expected in the new arrangement of reactors?

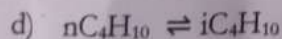
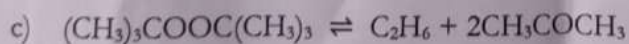
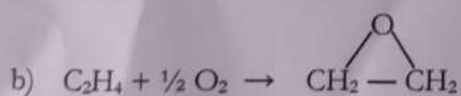
$$x_1 = 0$$

$$x_2 = 1$$

(5)

(25 Marks)

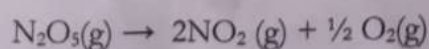
3. Write the rate law for the following reactions assuming each reaction follows an elementary rate law.



(20)

(20 Marks)

4. The activation energy for the reaction below equals $1.0 \times 10^5 \text{ J/mol}$. Given $k = 2.5 \times 10^{-3} \text{ sec}^{-1}$ at 332 K, find k at 375 K.

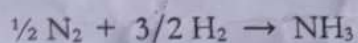


(5)

Based on information, find the temperature at which k is twice as large as it is at 332K.

(10 Marks)

5. The gas-phase reaction is to be carried out isothermally. The molar feed is 50% H_2 , and 50% N_2 , at a pressure of 16.4 atm and 227°C.



(a) Construct a complete stoichiometric table.

(b) What are CA_0 , δ and ϵ ? Calculate the concentrations of ammonia and hydrogen when the conversion of H_2 is 60%.

(c) Suppose by chance the reaction is elementary with $K_{N_2} = 40 \text{ dm}^3/\text{mol.s}$, Write the rate of reaction as a function of conversion for (1) a flow system and (2) a constant volume batch system.

(25 Marks)

Examiner's Name
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