

# **MANICALAND STATE UNIVERSITY OF APPLIED SCIENCES**

**FACULTY OF ENGINEERING**

**Chemical and Processing Engineering Department**

**CHEMICAL REACTION ENGINEERING I**

**CODE: HCHE 221**

**SESSIONAL EXAMINATIONS**

**APRIL-MAY 2021**

**DURATION: 3 HOURS**

**EXAMINER: DR M. CHIGONDO**

## **INSTRUCTIONS**

1. *Answer **all** questions*
2. *Each question carries 25 marks*
3. *Total marks 100*

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## **QUESTION ONE**

- (a) Differentiate *elementary* and *non-elementary reactions*. [2]
- (b) On doubling the concentration of a reactant, the rate of reaction triples. Find the reaction order. [2]
- (c) With the aid of an illustration define fractional conversion,  $X_A$  [2]
- (d) For an irreversible gas phase reaction  $3A \rightarrow 5R$ , determine the value of  $\mathcal{E}_A$  if the feed is a mixture of 60% A and 40% inert. [3]
- (e) Acetaldehyde ( $\text{CH}_3\text{CHO}$ ) decomposes in a batch reactor operating at  $520^\circ\text{C}$  and  $101\text{ kPa}$ . The reaction stoichiometry is  $\text{CH}_3\text{CHO} (g) \rightarrow \text{CH}_4 (g) + \text{CO}(g)$ . Under these conditions the reaction is known to be irreversible with a rate constant of  $430\text{ cm}^3/\text{mol sec}$ . If  $100\text{ g/s}$  of acetaldehyde is fed to the reactor, determine the reactor volume necessary to achieve 35% decomposition. [7]
- (f) The schematic reaction  $A + B \rightarrow P$  is assumed to consist of two elementary steps:
1.  $A + B \rightarrow A^* + B$  (forward reaction rate =  $k_1$ ; reverse reaction rate =  $k_{-1}$ )
  2.  $A^* \rightarrow P$  (forward reaction rate =  $k_2$ ). Show that using steady state approximation  $d[P]/dt = (k_1 k_2 [A] [b]) / (k_{-1}[B] + k_2)$ . [5]
- (g) For a gas reaction at  $400\text{ K}$ , the rate is reported as

$$\frac{dp_A}{dt} = 3.0 p_A^2 \text{ atm/h}$$

(i) What are the units of the rate constant? [2]

(ii) What is the value of the rate constant for this reaction if the rate equation is written as:

$$r_A = \frac{-1}{V} \frac{dNA}{dt} = k C_A^2, \text{ mol/l.h} \quad [2]$$

## QUESTION TWO

(a) (i) Define the term 'specific reaction rate' or 'rate of reaction'. [1]

(ii) Given that:



(b) A 2 liter per minute of liquid containing A and B ( $C_{Ao} = 0.30 \text{ mol/liter}$ ,  $C_{Bo} = 0.05 \text{ mol/liter}$ ) flow into a mixed reactor of volume,  $V = 1 \text{ liter}$ . The materials react in a complex manner for which the stoichiometry is unknown. The outlet stream from the reactor contains A, B, and C ( $C_{Af} = 0.08 \text{ mol/litre}$ ,  $C_{Bf} = 0.07 \text{ mol/litre}$ ,  $C_{Cf} = 0.03 \text{ mol/liter}$ ). Find the rate of reaction of A, B, and C for the conditions within the reactor. [5]

(c) (i) What is a *mixed flow reactor*? [1]

(ii) State **two** advantages of a mixed flow reactor. [2]

(d) A mixed flow reactor is used to determine the kinetics of a reaction whose stoichiometry  $A \rightarrow R$ . The flow rate of an aqueous solution of  $100 \text{ mol A/L}$  to a  $1 \text{ litre}$  reactor are used and for each run and outlet concentration of A is measured. Find the rate equation to represent the following data:

$V_o/\text{L/min}$	1	3	12
$C_A/\text{mol/L}$	2	10	25

[10]

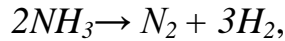
(e) Define  $\varepsilon_A$  [1]

- (ii) Which two reactor types performance is identical for constant density systems? [2]

### QUESTION THREE

- (a) State any **three** different factors to be considered for reactor design? [3]
- (b) With the aid of equations distinguish between *holding time* and *space time* [4]

- (c) At 76 °C  $NH_3$  decomposes as follows:



determine the size of PFR operating at 75 °C and 200 atm needed for 75 % conversion of 10 mol/h  $NH_3$  in a 0.67  $NH_3$  and 0.33 inert feed. [8]

- (d) A specific enzyme acts as a catalyst in fermentation of reactant A. At a given enzyme concentration in aqueous feed of 20 L /min, find the volume of the MFR needed for 90 % conversion of reactant A ( $C_{A0} = 2 \text{ mol/L}$ ). The kinetics of the fermentation reaction at this enzyme concentration is given by:

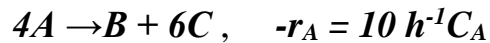


- (e) (i) What are *multiple reactions*? [1]
- (ii) State any **two** classes of such reactions [2]

### QUESTION FOUR

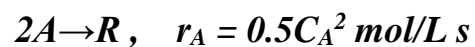
- (a) State the differences between *differential* and *integral* method of analysis of batch reactor data. [7]

(b) At 300 °C a substance A decomposes as follows:



Find the size of the MFR operating at 700 °C and 11.4 atm needed for 70 % conversion of 10 mol/h of A in a 70% A and 30 % inerts feed [7]

(c) The gaseous feed of pure A (1 mol/L) enters a mixed flow reactor of volume 4 liters and reacts as follows



(i) What is the order of this reaction?

(ii) Calculate the feed rate in liters/min of the outlet concentration given that

$$C_A = 0.5 \text{ mol/L} \quad [5]$$

(d) With the aid of diagram show the different types of semi-batch reactors. [6]

**END OF EXAM**

## TABLE OF FORMULAE

### BATCH REACTOR

$$t = N_{A0} \int_0^{X_A} \frac{dX_A}{-r_A V}$$

$$t = C_{A0} \int_0^{X_A} \frac{dX_A}{-r_A} = - \int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A}$$

$$\tau = N_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A) V_0 (1 + \epsilon_A X_A)} = C_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A) (1 + \epsilon_A X_A)}$$

### MIXED FLOW REACTOR

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \frac{\Delta X_A}{-r_A} = \frac{X_A}{-r_A}$$

or

$$\frac{V}{F_{A0}} = \frac{\Delta X_A}{(-r_A) f} = \frac{X_{Af} - X_{Ai}}{(-r_A) f}$$

$$\frac{V}{F_{A0}} = \frac{X_A}{-r_A} = \frac{C_{A0} - C_A}{C_{A0} (-r_A)}$$

$$\tau = \frac{1}{s} = \frac{V}{v_0} = \frac{V C_0}{F_{A0}} = \frac{C_{A0} X_A}{-r_A}$$

or

$$\tau = \frac{V C_0}{F_{A0}} = \frac{C_{A0} (X_{Af} - X_{Ai})}{(-r_A) f}$$

or

$$\tau = \frac{V}{v} = \frac{C_{A0} X_A}{-r_A} = \frac{C_{A0} - C_A}{-r_A}$$

### PLUG FLOW REACTOR

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A}$$

$$\tau = \frac{V}{v_0} = C_{A0} \int_0^{X_{Af}} \frac{dX_A}{-r_A}$$

$$\frac{V}{F_{A0}} = \frac{V}{C_{A0} v_0} = \int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{-r_A}$$

$$\tau = \frac{V}{v_0} = C_{A0} \int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{-r_A}$$

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A} = - \frac{1}{C_{A0}} \int_{A0}^{X_{Af}} \frac{dC_A}{-r_A}$$

$$\tau = \frac{V}{v_0} = C_{A0} \int_0^{X_{Af}} \frac{dX_A}{-r_A} = - \int_{A0}^{X_{Af}} \frac{dC_A}{-r_A}$$

$$X_A = 1 - \frac{C_A}{C_{A0}} \quad \text{and} \quad dX_A = - \frac{dC_A}{C_{A0}}$$

### BATCH REACTOR

$$t = N_{A0} \int_0^{X_A} \frac{dX_A}{-r_A V}$$

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$$\tau = N_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A) V_0 (1 + \varepsilon_A X_A)} = C_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A) (1 + \varepsilon_A X_A)}$$

### MIXED FLOW REACTOR

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \frac{\Delta X_A}{-r_A} = \frac{X_A}{-r_A}$$

or

$$\frac{V}{F_{A0}} = \frac{\Delta X_A}{(-r_A) f} = \frac{X_{Af} - X_{Ai}}{(-r_A) f}$$

$$\frac{V}{F_{A0}} = \frac{X_A}{-r_A} = \frac{C_{A0} - C_A}{C_{A0} (-r_A)}$$

$$\tau = \frac{1}{s} = \frac{V}{v_0} = \frac{V C_0}{F_{A0}} = \frac{C_{A0} X_A}{-r_A}$$

or

$$\tau = \frac{V C_0}{F_{A0}} = \frac{C_{A0} (X_{Af} - X_{Ai})}{(-r_A) f}$$

or

$$\tau = \frac{V}{v} = \frac{C_{A0} X_A}{-r_A} = \frac{C_{A0} - C_A}{-r_A}$$

### PLUG FLOW REACTOR

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A}$$

$$\frac{V}{F_{A0}} = \frac{V}{C_{A0} v_0} = \int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{-r_A}$$

$$\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int_0^{X_{Af}} \frac{dX_A}{-r_A} = - \frac{1}{C_{A0}} \int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A}$$

$$\tau = \frac{V}{v_0} = C_{A0} \int_0^{X_{Af}} \frac{dX_A}{-r_A} = - \int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A}$$

$$X_A = 1 - \frac{C_A}{C_{A0}} \quad \text{and} \quad dX_A = - \frac{dC_A}{C_{A0}}$$

$$\tau = \frac{V}{v_0} = C_{A0} \int_0^{X_{Af}} \frac{dX_A}{-r_A}$$

$$\tau = \frac{V}{v_0} = C_{A0} \int_{X_{Ai}}^{X_{Af}} \frac{dX_A}{-r_A}$$

Performance Equations for  $n$ th-order Kinetics and  $\varepsilon_A \neq 0$

	Plug Flow	Mixed Flow
$n = 0$ $-r_A = k$	$\frac{k\tau}{C_{A0}} = X_A$	$\frac{k\tau}{C_{A0}} = X_A$
$n = 1$ $-r_A = kC_A$	$k\tau = (1 + \varepsilon_A) \ln \frac{1}{1 - X_A} - \varepsilon_A X_A$	$k\tau = \frac{X_A(1 + \varepsilon_A X_A)}{1 - X_A}$
$n = 2$ $-r_A = kC_A^2$	$k\tau C_{A0} = 2\varepsilon_A(1 + \varepsilon_A) \ln(1 - X_A) + \varepsilon_A^2 X_A + (\varepsilon_A + 1)^2 \frac{X_A}{1 - X_A}$	$k\tau C_{A0} = \frac{X_A(1 + \varepsilon_A X_A)^2}{(1 - X_A)^2}$
any $n$ $-r_A = kC_A^n$		$k\tau C_{A0}^{n-1} = \frac{X_A(1 + \varepsilon_A X_A)^n}{(1 - X_A)^n}$
$n = 1$ $A \xrightarrow[\frac{1}{2}]{1} R$ $C_{R0} = 0$	$\frac{k\tau}{X_{Ae}} = (1 + \varepsilon_A X_{Ae}) \ln \frac{X_{Ae}}{X_{Ae} - X_A} - \varepsilon_A X_A$	$\frac{k\tau}{X_{Ae}} = \frac{X_A(1 + \varepsilon_A X_A)}{X_{Ae} - X_A}$
General expression	$\tau = C_{A0} \int_0^{X_A} \frac{dX_A}{-r_A}$	$\tau = \frac{C_{A0} X_A}{-r_A}$

Performance Equations for  $n$ th-order Kinetics and  $\varepsilon_A = 0$

	Plug Flow or Batch	Mixed Flow
$n = 0$ $-r_A = k$	$\frac{k\tau}{C_{A0}} = \frac{C_{A0} - C_A}{C_{A0}} = X_A$	$\frac{k\tau}{C_{A0}} = \frac{C_{A0} - C_A}{C_{A0}} = X_A$
$n = 1$ $-r_A = kC_A$	$k\tau = \ln \frac{C_{A0}}{C_A} = \ln \frac{1}{1 - X_A}$	$k\tau = \frac{C_{A0} - C_A}{C_A} = \frac{X_A}{1 - X_A}$
$n = 2$ $-r_A = kC_A^2$	$k\tau C_{A0} = \frac{C_{A0} - C_A}{C_A} = \frac{X_A}{1 - X_A}$	$k\tau = \frac{(C_{A0} - C_A)}{C_A^2} = \frac{X_A}{C_{A0}(1 - X_A)^2}$
any $n$ $-r_A = kC_A^n$	$(n - 1)C_{A0}^{n-1} k\tau = \left(\frac{C_A}{C_{A0}}\right)^{1-n} - 1 = (1 - X_A)^{1-n} - 1$	$k\tau = \frac{C_{A0} - C_A}{C_A^n} = \frac{X_A}{C_{A0}^{n-1}(1 - X_A)^n}$
$n = 1$ $A \xrightarrow[\frac{1}{2}]{1} R$ $C_{R0} = 0$	$k_1\tau = \left(1 - \frac{C_{Ae}}{C_{A0}}\right) \ln \left(\frac{C_{A0} - C_{Ae}}{C_A - C_{Ae}}\right) = X_{Ae} \ln \left(\frac{X_{Ae}}{X_{Ae} - X_A}\right)$	$k_1\tau = \frac{(C_{A0} - C_A)(C_{A0} - C_{Ae})}{C_{A0}(C_A - C_{Ae})} = \frac{X_A X_{Ae}}{X_{Ae} - X_A}$
General rate	$\tau = \int_{C_A}^{C_{A0}} \frac{dC_A}{-r_A} = C_{A0} \int_0^{X_A} \frac{dX_A}{-r_A}$	$\tau = \frac{C_{A0} - C_A}{-r_A} = \frac{C_{A0} X_A}{-r_A}$