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*

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 (CH_3CHO) decomposes in a batch reactor operating at 520 ^oC and *101 kPa*. The reaction stoichiometry is $CH_3CHO\ (g) \rightarrow CH_4\ (g) + CO(g)$. Under these conditions the reaction is known to be irreversible with a rate constant of 430 cm^3/mol sec. If 100 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 → P is assumed to consist of two elementary steps:

1. A + B → A* + B (forward reaction rate = k_1; reverse reaction rate = k_{-1})
2. A* → P (forward reaction rate = k_2). Show that using steady state approximation d[P]/dt = (k_1k_2 [A] [b])/ (k_{-1}[B] +k_2). [5]

(g) For a gas reaction at 400 K, the rate is reported as

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

(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:

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

QUESTION TWO

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

(ii) Given that:

$4A + 3B \rightarrow 10\,C$, what is the relationship between r_A, r_B and r_C? [3]

(b) A *2* liter per minute of liquid containing A and B ($C_{Ao} = 0.30$ *mol/liter*, $C_{Bo} = 0.05$ mol/liter) flow into a mixed reactor of volume, $V = 1$ *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 ($C_{Af} = 0.08$ *mol/litre*, $C_{Bf} = 0.07$ *mol/litre*, $C_{Cf} = 0.03$ *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 mol A/L* to a *1 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/L/min	1	3	12
C_A/mol/L	2	10	25

[10]

(e) Define ε_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:

$2NH_3 \rightarrow N_2 + 3H_2$,

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_{Ao}= *2 mo/L*). The kinetics of the fermentation reaction at this enzyme concentration is given by:

A→R, $\quad r_A = \frac{0.1 C_A}{1+0.5\, C_A} \frac{mol}{liter.min}$ **[**7]

(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:

$$4A \rightarrow B + 6C\,, \quad -r_A = 10\ h^{-1}C_A$$

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

$$2A \rightarrow R\,, \quad r_A = 0.5C_A^2\ mol/L\ s$$

(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 mol/L [5]

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

END OF EXAM

TABLE OF FORMULAE

BATCH REACTOR

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

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

$$\tau = N_{AO} \int_o^{X_A} \frac{dX_A}{(-r_A)V_o(1+\varepsilon_A X_A)} = C_{AO} \int_o^{X_A} \frac{dX_A}{(-r_A)(1+\varepsilon_A X_A)}$$

MIXED FLOW REACTOR

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

$$\tau = \frac{1}{s} = \frac{V}{v_O} = \frac{VC_o}{F_{AO}} = \frac{C_{AO}X_A}{-r_A}$$

or

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

or

$$\tau = \frac{VC_o}{F_{AO}} = \frac{C_{AO}(X_{Af-}X_{Ai})}{(-r_A)f}$$

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

or

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

PLUG FLOW REACTOR

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

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

$$\frac{V}{F_{AO}} = \frac{V}{C_{AOvo}} = \int_{AI}^{X_{Af}} \frac{dX_A}{-r_A}$$

$$\tau = \frac{V}{v_O} = C_{AO} \int_{AI}^{X_{Af}} \frac{dX_A}{-r_A}$$

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

$$\tau = \frac{V}{v_O} = C_{AO} \int_0^{X_{AI}} \frac{dX_A}{-r_A} = -\int_{AO}^{X_{Af}} \frac{dC_A}{-r_A}$$

$X_A = 1 - \frac{C_A}{C_{AO}}$ **and** $dX_A = -\frac{dC_A}{C_{AO}}$

BATCH REACTOR

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

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

$$\tau = N_{AO}\int_o^{X_A} \frac{dX_A}{(-r_A)V_o(1+\varepsilon_A X_A)} = C_{AO}\int_o^{X_A} \frac{dX_A}{(-r_A)(1+\varepsilon_A X_A)}$$

MIXED FLOW REACTOR

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

$$\tau = \frac{1}{s} = \frac{V}{v_O} = \frac{VC_o}{F_{AO}} = \frac{C_{AO}X_A}{-r_A}$$

or

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

or

$$\tau = \frac{VC_o}{F_{AO}} = \frac{C_{AO}\left(X_{Af-}X_{Ai}\right)}{(-r_A)f}$$

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

or

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

PLUG FLOW REACTOR

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

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

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$$\tau = \frac{V}{v_O} = C_{AO}\int_0^{X_{AI}} \frac{dX_A}{-r_A} = -\int_{AO}^{X_{Af}} \frac{dC_A}{-r_A}$$

$X_A = 1 - \frac{C_A}{C_{AO}}$ **and** $dX_A = -\frac{dC_A}{C_{AO}}$

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

	Plug Flow	Mixed Flow
$n = 0$ $-r_A = k$	$\frac{k\tau}{C_{A0}} = X_A$	$\frac{k\tau}{C_{A0}} = X_A$
$n = 1$ $-r_A = kC_A$	$k\tau = (1 + \varepsilon_A)\ln\frac{1}{1 - X_A} - \varepsilon_A X_A$	$k\tau = \frac{X_A(1 + \varepsilon_A X_A)}{1 - X_A}$
$n = 2$ $-r_A = kC_A^2$	$k\tau C_{A0} = 2\varepsilon_A(1 + \varepsilon_A)\ln(1 - X_A) + \varepsilon_A^2 X_A + (\varepsilon_A + 1)^2 \cdot \frac{X_A}{1 - X_A}$	$k\tau C_{A0} = \frac{X_A(1 + \varepsilon_A X_A)^2}{(1 - X_A)^2}$
any n $-r_A = kC_A^n$		$k\tau C_{A0}^{n-1} = \frac{X_A(1 + \varepsilon_A X_A)^n}{(1 - X_A)^n}$
$n = 1$ $A \underset{2}{\overset{1}{\rightleftarrows}} rR$ $C_{R0} = 0$	$\frac{k\tau}{X_{Ae}} = (1 + \varepsilon_A X_{Ae})\ln\frac{X_{Ae}}{X_{Ae} - X_A} - \varepsilon_A X_A$	$\frac{k\tau}{X_{Ae}} = \frac{X_A(1 + \varepsilon_A X_A)}{X_{Ae} - X_A}$
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 nth-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 $-r_A = kC_A^n$	$(n - 1)C_{A0}^{n-1}k\tau = \left(\frac{C_A}{C_{A0}}\right)^{1-n} - 1 = (1 - X_A)^{1-n} - 1$	$k\tau = \frac{C_{A0} - C_A}{C_A^n} = \frac{X_A}{C_{A0}^{n-1}(1 - X_A)^n}$
$n = 1$ $A \underset{2}{\overset{1}{\rightleftarrows}} R$ $C_{R0} = 0$	$k_1\tau = \left(1 - \frac{C_{Ae}}{C_{A0}}\right)\ln\left(\frac{C_{A0} - C_{Ae}}{C_A - C_{Ae}}\right) = X_{Ae}\ln\left(\frac{X_{Ae}}{X_{Ae} - X_A}\right)$	$k_1\tau = \frac{(C_{A0} - C_A)(C_{A0} - C_{Ae})}{C_{A0}(C_A - C_{Ae})} = \frac{X_A X_{Ae}}{X_{Ae} - X_A}$
General rate	$\tau = \int_{C_A}^{C_{A0}}\frac{dC_A}{-r_A} = C_{A0}\int_0^{X_{Ae}}\frac{dX_A}{-r_A}$	$\tau = \frac{C_{A0} - C_A}{-r_{Af}} = \frac{C_{A0}X_A}{-r_{Af}}$