MANICALAND STATE UNIVERSITY OF APPLIED SCIENCES

FACULTY OF ENGINEERING

CHEMICAL AND PROCESSING ENGINEERING DEPARTMENT

CHEMICAL REACTION ENGINEERING I

CODE: HCHE 221

SESSIONAL EXAMINATIONS
OCTOBER 2021

DURATION: 3 HOURS

EXAMINER: DR M. CHIGONDO

INSTRUCTIONS

1. *Answer **all** questions in **Section** A*
2. *Answer f**our** questions from **Section B***
3. *Total marks 100*

Section A:

Question 1

(a) Define the following:

(i) *rate of reaction*

(ii) *rate constant*

(iii) *reaction mechanism*

(iv) *order of reaction* [4]

(b) 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]

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

(i) $r_A = \frac{-1}{V}\frac{dNA}{dt} = k\ C_A^2$, mol/L.h [2]

(ii) $r_A = k\ C_A^2$, mol/m^3.s [2]

Question 2

(a) In a reaction between A and B, the initial rate of reaction (r_0) was measured for different initial concentrations of A and B as given in Table 1.

Table 1

A/ mol L^{-1}	0.2	0.2	0.4
B/ mol L^{-1}	0.3	0.1	0.05
r_0/mol L^{-1}s^{-1}	5.07×10^{-5}	5.07×10^{-5}	1.43×10^{-4}

What is the order of the reaction with respect to *A* and *B*? [5]

(b) Consider a certain reaction $A \rightarrow Products$ with $k = 2.0 \times 10^{-2}\ s^{-1}$. Calculate the concentration of *A* remaining after 100 s if the initial concentration of *A* is 1.0 mol L^{-1} [3]

(c) Aqueous *A* reacts to form *R* *(A→R)* and in the first minute in MFR its concentration drops from $C_{AO} = 2.03$ to $C_M = 1.97$ mol/L.

Find: (i) the rate equation for the reaction if the kinetics are second order with respect to A. [5]

(ii) the conversion after 5 minutes. [2]

Question three

(a) The schematic reaction $A + M \rightarrow P$ is assumed to consist of two elementary steps:

1. $A + M \rightarrow A^* +$ M (forward reaction rate = k_1;
2. reverse reaction rate = k_{-1})

$A^* \rightarrow P$ (forward reaction rate = k_2). Show that using steady state approximation

$$\frac{d[P]}{dt} = \frac{k1k2\ [A]\ [M])}{k_{-1}[M] + k_2).}$$ [5]

A liquid feed of 66.6% A and 33.3% inert enters a CSTR at 27 °C, 580 kPa and at a flow rate of 55 L/min, which is operated adiabatically. The reaction $A \rightarrow B + C$ is an elementary irreversible reaction. Calculate the volume necessary to achieve 90% conversion [5]

(b) Reactant A decomposes as follows

$3A \rightarrow B_4 + 2C_2$

At a given instant, the rate of decomposition of A is 1.0 x 10^{-3} *mol*/Ls

(i) Express the rate in three different ways using the differential notation [3]

(ii) determine the rate of formation of B_4 and of C_2 [2]

Section B:

Answer any **four** questions, each question carries 20 marks

Question four

(a) (i) What are multiple reactions? [1]

(ii) Explain. [2]

(b) A homogeneous gas phase reaction $A \rightarrow 3R$ satisfactorily follows second order kinetics. For a feed rate 4 m^3/h of pure A 350 °C and 5 atm, an experimental reactor (25 mm ID pipe x 2 mm long) gives 60 % conversion of feed. A commercial plant is to handle 320 m^3/h of feed containing 50 % A and 50 % inerts at 350 °C and 25 atm obtaining 80 % conversion of *A*.

(i) how many 2 m lengths of 25 mm ID pipe are required? [5]

(ii) Should they be parallel or in series [5]

(Assume plug flow in pipe and ideal gas behavior)

(c) Write brief notes on the following types of reactors:

(ii) CSTR [3]

(iii) Plug Flow Reactor. [4]

Question five

(a) What is a batch reactor? [1]

(b) What are the advantages and disadvantages of a batch reactor? [5]

(c) An aqueous concentration is introduced into a batch reactor where it reacts away to form product *R* according to stoichiometry $A \rightarrow R$. The concentration of *A* in the reactor is monitored at various rates as shown in Table 2.

Table 2

Time (min)	0	100	200	300	400
C_A (mol/m^3	1000	500	333	250	200

Given that C_{Ao} = 500 mol/m^3.

Determine (i) the conversion after 5 hours

(ii) rate equation to fit the data [5]

(d) A gaseous reactant A decomposes as follow:

$\boldsymbol{A \rightarrow 4R}$, $r_A = (0.6 min^{-1})\, C_A$

Find the conversion of A in a 50% A – 50 % inert feed (v_o = 90 L/min, C_A = 150 mmol/L) to 0.5 dm^3 MFR reactor. [5]

(e) (i) What is a *semi-batch reactor*?

(ii) With the aid of diagram show the different types of semi-batch reactors

[4]

Question six

(a) A flow rate of F_{AO} = 1 L/s of 10% ozone -90% air mixture at a total pressure of 1.5 atm and 93 °C passes through a reactor. Under these conditions ozone decomposes as follows

$2O_3 \rightarrow 3O_2$ with the second order rate, $r_{O3} = 0.05C_{O3}^2\ mol/Ls$

$p_A = C_Ao$ RT [R = 0.0831 atm/ K mol]

i. Determine ε_A and C_{Ao} [3]

Find the residence time needed for 50% decomposition of ozone the size of a

1. PFR [4]
2. MFR [3]

(b) A gaseous high molecular weight compound A is fed continuously to a heated high temperature MFR where it thermally cracks into lower molecular weight materials, collectively called R, by a stoichiometry approximated by $A \rightarrow 5R$. By changing the feed rate, different extents of cracking are obtained as follows:

F_{Ao} mol/h	300	1000	3000	5000
C_{Aout} mol/L	16	30	50	60

V = 0.1 L, C_{AO} = 100 mol/L.

Find the rate equation that represents the cracking [10]

Question seven

a. Explain the elementary and non-elementary reactions. [2]

b. State **four** factors to be considered for reactor design [4]

c. Define *space time* and *space velocity* [2]

d. 1 liter per minute of liquid containing A and B (C_{AO} = 0.10 mol/L, C_{BO} = 0.01 mol/L) flow into a mixed reactor of volume V = 2 liters. 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} = 0.02 mol/L, C_{Bf} = 0.03 moll/L, C_{Cf} = 0.04 mol/L), Find the rate of reaction of A, B and C for the conditions within the reactor. [6]

e. A specific enzyme acts as a catalyst in fermentation of reactant *A*. At a given enzyme concentration in aqueous feed of 25 L/min, find the volume of the MFR reactor 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, $\mathbf{r_A} = \frac{0.1 C_A}{1+0.5\, C_A} \frac{mol}{liter.min}$ [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 $dX_A = -\frac{dC_A}{C_{AO}}$

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	$\tau = \int_{C_A}^{C_{A0}}\frac{dC_A}{-r_A} = C_{A0}\int_0^{X_{Ae}}\frac{dX_A}{-r_A}$	$\tau = \frac{C_{A0}-C_A}{-r_{Af}} = \frac{C_{A0}X_A}{-r_{Af}}$