MANICALAND STATE UNIVERSITY OF APPLIED SCIENCES

FACULTY OF ENGINEERING

CHEMICAL AND PROCESSING ENGINEERING DEPARTMENT

REACTOR ANALYSIS AND DESIGN I/CHEMICAL REACTION ENGINEERING I

CODE: CHEP 214/HCHE 221

SESSIONAL EXAMINATIONS

DECEMBER 2022

DURATION: 3 HRS
LECTURER: DR M. CHIGONDO

INSTRUCTIONS

1. *Answer **all** questions*
2. *The paper consists of 7 printed pages*
3. *Total marks 100*

Additional materials: graph paper

Question one

(a) Define the term ‘specific reaction *rate of reaction* [1]

(b) (i) The rate equation of a reaction $2A + B \rightarrow C$ is $-r_A = k\,CA^2\,C_B$. Find the unit of ‘*k*’. [2]

(ii) A certain reaction has a rate given by $-r_A = 0.003C_A^2$, mol/cm^3-min. If the concentration is to be expressed in mol/liter and time in hours, what would be the value and units of the rate constant? [3]

(c) Define the terms *molecularity* and *order* of an elementary reaction [2]

(d) Distinguish between *homogeneous* and *heterogeneous* reactions. [2]

(e) **A mixed flow** reactor is being used to determine the kinetics of a reaction whose stoichiometry is A →R. For this purpose, various flow rates of an aqueous solution of 100 mol A /L are fed to a 1-liter reactor, and for each run the outlet concentration of A is measured (**Table 1**). Find a rate equation to represent the following data. Also assume that reactant alone affects the rate.

Table 1

$\mathbf{v_0}$ (litre/min)	1	6	24
C_A (mol/litre)	2	10	25

[10]

(f) The primary reaction occurring in the homogeneous decomposition of nitrous oxide is found to be $N_2O \rightarrow N_2 + \frac{1}{2} O_2$ with rate

$r_{N_2O} = \frac{k_l\,[N_2O]_2}{1 + k_1[N_2O]}$. Devise a mechanism to explain the observed rate [5]

2. (a) Differentiate between *differential* and *integral* method of analysis of batch rector data. [7]

(b) At 700 ºC, *A* decomposes as follows :

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

Find the size of the plug flow reactor operating at 700 ºC and 11.4 atm needed for 75 % conversion of 10 mol/h of *A* in a 90% *A* and 10 % inerts feed. [7]

(c) The gaseous feed of pure A (1 mol/L) enters a mixed flow reactor of volume 2 liters and reacts as follows

$$2A \rightarrow R, \quad r_A = 0.25C_A^2 \text{ mol/L s}$$

(i) What is the order of this reaction?

(ii) Calculate the feed rate in liters /min of the outlet concentration $C_A = 0.25$ mol/L [5]

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

Question three

(a) State **three** factors to be considered for reactor design [3]

(b) With the aid of equations distinguish between *holding time* and *space time* for flow reactors [4]

(c) For an irreversible gas phase reaction 2A→ 5R, determine the value of ε_A if the feed is a mixture of 85% A and 15% inert. [3]

(d)(i) What is a *batch reactor*? [1]

(ii) State the advantages and disadvantages of a batch reactor? [5]

(iii) Differentiate between MFR and PFR. [4]

(e) The polymerization of a monomer M in made in a MFR. Given that $v_o = 1.2\ L/h$, $C_{AO} = 3\ mol/h$ and 80 % conversion is achieved, calculate the volume of the reactor. Give that $r_M = 6.33X\ 10^{-2}\ C_A$ [5]

Question four

(a) State **three** factors that make up the contacting or flow in non-ideal reactors [3]

(b) A batch of radioactive material is dumped into a river. At a dam, about 200 km downstream the flowing waters (3000 m^3/s) are monitored for a particular radioisotope ($t_{1/2}$ > 10 yr) and the data of **Fig. 1** are obtained.

(i) How many units of this tracer were introduced into the river? [3]

(ii) What is the volume of river waters between the dam and the point of introduction of tracer? [3]

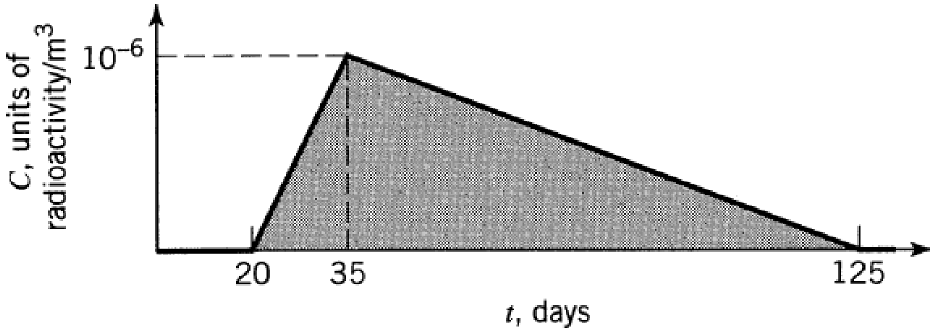

Fig. 1

(c) A flow rate of F_{AO} = 1 L/s of 20 % ozone -80 % air mixture at a total pressure of 1.5 atm and 93 °C passes through a plug flow reactor (PFR). Under these conditions ozone decomposes as follows

$2O_3 \rightarrow 3O_2$ with the second order rate**,** $r_{O3} = 0.05\ C^2_{O3}$ (mol/Ls).

(i)Write the formula of the residence time for a PFR [1]

(ii) Find the ε_A for the reaction [2]

(iii) Find the residence time of the size of the PFR needed for 50 % decomposition of ozone.

$$\boldsymbol{p_A = C_{Ao}}\ \mathbf{RT} \quad \mathbf{,[R = 8.31}\ \mathbf{N}\mathrm{m/mol}\ \mathbf{K\ ,\ T\ is\ in\ K}]$$ [7]

(d) (i) Given that:
$4A + 3B \rightarrow 10\ C$, what is the relationship between r_A, r_B and r_C? [3]

(ii) 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. [3]

END OF EXAM

LIST 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

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

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

or

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

PLUG FLOW REACTOR

$$\frac{V}{F_{AO}} = \frac{\tau}{C_{AO}} = \int_{0}^{X_{Af}} \frac{dX_A}{-r_A}$$

$$\tau = \frac{V}{v_O} = C_{AO} \int_{0}^{X_{Af}} \frac{dX_A}{-r_A}$$

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

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

$$\frac{V}{F_{AO}} = \frac{\tau}{C_{AO}} = \int_{0}^{X_{Af}} \frac{dX_A}{-r_A} = -\frac{1}{C_{AO}} \int_{AO}^{X_{Af}} \frac{dC_A}{-r_A}$$

$$\tau = \frac{V}{v_O} = C_{AO} \int_{0}^{X_{AI}} \frac{dX_A}{-r_A} = -\int_{AO}^{X_{Af}} \frac{dC_A}{-r_A}$$

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

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

	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 $-r_A = kC_A^n$	$(n-1)C_{A0}^{n-1}k\tau = \left(\frac{C_A}{C_{A0}}\right)^{1-n} - 1 = (1 - X_A)^{1-n} - 1$	$k\tau = \frac{C_{A0} - C_A}{C_A^n} = \frac{X_A}{C_{A0}^{n-1}(1 - X_A)^n}$
$n = 1$ $A \underset{2}{\overset{1}{\rightleftharpoons}} R$ $C_{R0} = 0$	$k_1\tau = \left(1 - \frac{C_{Ae}}{C_{A0}}\right) \ln \left(\frac{C_{A0} - C_{Ae}}{C_A - C_{Ae}}\right) = X_{Ae} \ln \left(\frac{X_{Ae}}{X_{Ae} - X_A}\right)$	$k_1\tau = \frac{(C_{A0} - C_A)(C_{A0} - C_{Ae})}{C_{A0}(C_A - C_{Ae})} = \frac{X_A X_{Ae}}{X_{Ae} - X_A}$
General rate	$\tau = \int_{C_A}^{C_{A0}} \frac{dC_A}{-r_A} = C_{A0} \int_0^{X_{Ae}} \frac{dX_A}{-r_A}$	$\tau = \frac{C_{A0} - C_A}{-r_{Af}} = \frac{C_{A0} X_A}{-r_{Af}}$

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 $-r_A = kC_A^n$		$k\tau C_{A0}^{n-1} = \frac{X_A(1 + \varepsilon_A X_A)^n}{(1 - X_A)^n}$
$n = 1$ $A \underset{2}{\overset{1}{\rightleftharpoons}} rR$ $C_{R0} = 0$	$\frac{k\tau}{X_{Ae}} = (1 + \varepsilon_A X_{Ae})\ln \frac{X_{Ae}}{X_{Ae} - X_A} - \varepsilon_A X_A$	$\frac{k\tau}{X_{Ae}} = \frac{X_A(1 + \varepsilon_A X_A)}{X_{Ae} - X_A}$
General expression	$\tau = C_{A0} \int_0^{X_A} \frac{dX_A}{-r_A}$	$\tau = \frac{C_{A0} X_A}{-r_A}$

$$\left(\begin{matrix}\text{Area under the} \\ C_{\text{pulse}}\text{ curve}\end{matrix}\right): \quad A = \int_0^\infty C\,dt \cong \sum_i C_i \Delta t_i = \frac{M}{v} \quad \left[\frac{\text{kg} \cdot \text{s}}{\text{m}^3}\right]$$

$$\left(\begin{matrix}\text{Mean of the} \\ C_{\text{pulse}}\text{ curve}\end{matrix}\right): \quad \bar{t} = \frac{\int_0^\infty tC\,dt}{\int_0^\infty C\,dt} \cong \frac{\sum_i t_i C_i \Delta t_i}{\sum_i C_i \Delta t_i} = \frac{V}{v} \quad [\text{s}]$$