Universiti Tun Hussein Onn Malaysia

UNIVERSITI TUN HUSSEIN ONN MALAYSIA

FINAL EXAMINATION
SEMESTER II
SESSION 2022/2023

COURSE NAME	:	CHEMICAL REACTION ENGINEERING
COURSE CODE	:	BNQ 20304
PROGRAMME CODE	:	BNN
EXAMINATION DATE	:	JULY / AUGUST 2023
DURATION	:	3 HOURS
INSTRUCTION	:	1. ANSWER **ALL** QUESTIONS 2. THIS FINAL EXAMINATION IS CONDUCTED VIA **CLOSE BOOK** 3. STUDENTS ARE **PROHIBITED** TO CONSULT THEIR OWN MATERIAL OR ANY EXTERNAL RESOURCES DURING THE EXAMINATION CONDUCTED VIA CLOSED BOOK

THIS QUESTION PAPER CONSISTS OF **SEVEN (7)** PAGES

Q1 The elementary gas phase reaction can be carried out in different types of reactors. The following gas-phase reaction is carried out in a 20 dm^3 constant-volume batch reactor. A pure reactant is initially placed in the reactor. Given that the rate of disappearance of CH_3CHO is 6 $mol/dm^3.s$

$$CH_3CHO \rightarrow CH_4 + CO$$

(a) State the rate of formation of CH_3CHO and the rate of disappearance of CH_4 and CO.
(3 marks)

(b) Determine the time to consume 99% moles of CH_3CHO if the reaction is first order with $k = 0.23\ min^{-1}$.
(4 marks)

(c) If a similar reaction is carried out in a CSTR-PFR flow reactor, calculate the volume of CSTR and PFR when the concentration of reactant is reduced to 1% of the initial concentration. The volumetric flow rate is 10 dm^3/hr and $k = 0.0001\ s^{-1}$.
(7 marks)

(d) Differentiate between batch and semi-batch reactors.
(4 marks)

(e) Based on the following data in **Table Q1(e),** examine over what range of conversions would the CSTR and PFR reactor volumes be identical.

Table Q1(e)

X	**0**	**0.2**	**0.4**	**0.5**	**0.6**	**0.8**	**0.9**
$-r_A$ ($mol/dm^3.min$)	1	1.67	5	5	5	1.25	0.91

(7 marks)

Q2 Polysyntech Pte. Ltd. company has been producing tyrene (B) from butylene (A), which are both in liquid forms using a CSTR, followed by a PFR. Daily reports show that the intermediate conversion is 40% and the second reactor maintained approximately up to 80% conversion is achieved using this reactors arrangement. However, the conversion drops for certain days before maintained up to 80%. Based on the data obtained during laboratory experiment in **Table Q2**, the process engineer found that, the maximum conversion for this reaction achieved is 90% with first order reaction. Thus, the company aims to increase the conversion. However, the suitable proper arrangement of reactors to achieve the maximum conversion yet to be decided.

Table Q2

X	**0**	**0.2**	**0.4**	**0.6**	**0.8**	**0.9**
$-r_A$ ($mol/dm^3.min$)	10	16.67	50	50	12.5	9.09

(a) Suggest the possible arrangement of reactors in series to achieve the maximum conversion, 90%, with the molar flow rate is 300 mol/min.
(19 marks)

(b) Identify **THREE (3)** possible reasons that cause the drop in conversion.

(6 marks)

Q3 The reaction is found to be an elementary reaction with the rate constant k is 0.24 liter/mol.s at 292 K. The feed to the reactor has the initial concentration of A at 2.0 mol/liter and the reaction is operated under constant operating temperature. Initial molar flow rate of reactant A is set up at 15 mol/s.

(a) Determine the order of the reaction corresponding to the rate constant.

(2 marks)

(b) Starting from general mole balance, express the design equation for an ideal isothermal CSTR in terms of conversion *X* with respect to reactant A.

(6 marks)

(c) Calculate the reactor volume required to achieve 75% conversion of reactant A.

(7 marks)

(d) The same reaction is now replaced in an ideal batch reactor of the same volume calculated in **Q3(b)**. Using your knowledge of design equation for an ideal isothermal batch reactor, evaluate the amount of time required to achieve the conversion up to 75% in a batch reactor.

(10 marks)

Q4 (a) The following liquid-phase reactions were carried out in a CSTR at 325 K.

$3A \rightarrow B + C$	$-r_{1A} = k_{1A}C_A$	$k_{1A} = 7.0\ min^{-1}$
$2C + A \rightarrow 3D$	$r_{2D} = k_{2D}C_C^2C_A$	$k_{2D} = 3.0\dfrac{dm^6}{mol^2 min}$
$4D + 3C \rightarrow 3E$	$r_{3E} = k_{3E}C_DC_C$	$k_{3E} = 2.0\dfrac{dm^3}{mol\ min}$

(i) Derive the net rates of formation for *A, B, C, D* and *E*.

(10 marks)

(ii) If the entry conditions for the CSTR are 100 dm^3/min and $C_{A0} = 3$, evaluate the reactor volume if the concentration inside the reactor were $C_A = 0.1$, $C_B = 0.93$, $C_c = 0.51$, $C_D = 0.049$ mol/dm^3.

(10 marks)

(b) Catalyst is something that lowers the activation energy of a reaction because of the activation energy is lower.

(i) Identify **TWO (2)** types of catalyst.

(2 marks)

(ii) Describe and illustrate the impact of reduced activation energy on the rate of a chemical reaction.

(3 marks)

- END OF QUESTIONS -

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

$$C_{A0} = \frac{P_{A0}}{RT_0} = \frac{y_{A0}P_0}{RT_0}$$

$$F_{A0} = C_{A0}\nu_0$$

$$V = \frac{F_{j0} - F_j}{-r_j} \text{ or } \frac{v_j C_{j0} - vC_j}{-r_j}$$

$$F_A = F_{A0}(1 - X)$$

$$\frac{dN_A}{dt} = r_A V$$

$$[N_A] = N_{A0}(1 - X)$$

$$t_1 = \int_{N_{A1}}^{N_{A0}} \frac{dN_A}{-r_A V}$$

$$\frac{(N_A/V_0)}{dt} = \frac{dC_A}{dt}$$

$$N_{A0}\frac{dX}{dt} = -r_A V$$

$$V = \int_{F_{j0}}^{F_j} \frac{dF_j}{r_j} = \int_{F_j}^{F_{j0}} \frac{dF_j}{-r_j}$$

$$\frac{F_{A0}dX}{dV} = -r_A$$

$$V = \frac{F_{A0}.X}{-r_A}$$

$$\frac{dF_A}{dV} = r_A$$

$$\int_{X_0}^{X_2} f(X)dX = \frac{h}{3}[f(X_0) + 4f(X_1) + f(X_2)]$$

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

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

$$[k] = \frac{(\text{Concetration})^{1-n}}{\text{time}}$$

$$r_{A,net} = r_{A,forward} + r_{B,reverse}$$

$$r_A \text{ reverse} = k_{-A} C_d^c C_D^d$$

$$r_A forward = -k_A C_A^a C_B^b$$

$$K_{equlibrium} = K_c = \frac{C_{Ce}^e C_{De}^d}{C_{Ae}^a C_{Be}^b}$$

$$\frac{-r_A}{a} = \frac{-r_B}{b} = \frac{r_C}{c} = \frac{r_D}{d}$$

$$C_B = \frac{N_B}{V} = \frac{N_{B0} - (b/a)N_{A0}X}{V}$$

$$= \frac{N_{A0}(\Theta - (b/a)X)}{V}$$

$$F_{B0} = F_{A0}\Theta_B$$

$$-\frac{b}{a}(F_{A0}X)$$

$$F_B = F_{A0}\left(\Theta_B - \frac{b}{a}X\right)$$

$$F_T = F_{T0} + F_{A0}.\delta.X$$

$$v = v_0(1 + y_{A0}\delta X)\frac{P_0}{P}\frac{T}{T_0}$$

$$= v_0(1 + \varepsilon X)\frac{P_0}{P}\frac{T}{T_0}$$

$$PV = ZR_T T$$

$$C_T = \frac{F_T}{v} = \frac{P}{ZRT}$$

$$\varepsilon = y_{A0}\delta$$

$$\left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1\right) = \delta$$

$$C_j = C_{T0}\left(\frac{F_j}{F_T}\right)$$

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$$\Theta_i = \frac{N_{i0}}{N_{A0}} = \frac{C_{i0}}{C_{A0}} = \frac{y_{i0}}{y_{A0}}$$

$$\text{Selectivity}(S_{D/U}) = \frac{r_D}{r_U} = \frac{\text{rate of formationof D}}{\text{rate of formationU}}$$

$$Y_D = \frac{r_D}{-r_A}$$

$$\widetilde{Y}_D = \frac{F_D}{F_{A0} - F_A}$$

$$r_A = r_D + r_U$$

$$r_A = k_D C_A^{\alpha_1} + k_U C_A^{\alpha_2}$$

$$S_{D/U} = \frac{r_D}{r_U} = \frac{k_D}{k_U} C_A^{\alpha_1 - \alpha_2}$$

$$S_{D/U} = \frac{r_D}{r_U} = \frac{k_D}{k_U} C_A^{\alpha_1 - \alpha_2} C_B^{\beta_1 - \beta_2}$$

$$r_{AD} = k_A \left(P_A C_\nu - \frac{C_{A\bullet S}}{K_A} \right)$$

$$\frac{P_A}{C_{A\bullet S}} = \frac{1}{K_A C_t} + \frac{P_A}{C_t}$$

$$C_{A\bullet S} = K_A P_A C_\nu$$

$$C_{C\bullet S} = \frac{(K_A P_A)^{1/2} C_t}{1 + 2(K_A P_A)^{1/2}}$$

$$R = \frac{8.314 \text{ kPa} \cdot \text{dm}^3}{\text{mol} \cdot \text{K}} \qquad R = \frac{1.987 \text{ Btu}}{\text{lb mol} \cdot {}^\circ\text{R}}$$

$$R = \frac{0.73 \text{ ft}^3 \cdot \text{atm}}{\text{lb mol} \cdot {}^\circ\text{R}} \qquad R = \frac{8.3144 \text{ J}}{\text{mol} \cdot \text{K}}$$

$$R = 0.082 \frac{\text{dm}^3 \cdot \text{atm}}{\text{mol} \cdot \text{K}} = \frac{0.082 \text{ m}^3 \cdot \text{atm}}{\text{kmol} \cdot \text{K}} \qquad R = \frac{1.987 \text{cal}}{\text{mol} \cdot \text{K}}$$

E = 82,000 cal/gmol

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$$\int_0^x \frac{dx}{1-x} = \ln\frac{1}{1-x}$$

$$\int_{x_1}^{x_2} \frac{dx}{(1-x)^2} = \frac{1}{1-x_2} - \frac{1}{1-x_1}$$

$$\int_0^x \frac{dx}{(1-x)^2} = \frac{x}{1-x}$$

$$\int_0^x \frac{dx}{1+\varepsilon x} = \frac{1}{\varepsilon}\ln(1+\varepsilon x)$$

$$\int_0^x \frac{1+\varepsilon x}{1-x}\,dx = (1+\varepsilon)\ln\frac{1}{1-x} - \varepsilon x$$

$$\int_0^x \frac{1+\varepsilon x}{(1-x)^2}\,dx = \frac{(1-\varepsilon)x}{1-x} - \varepsilon\ln\frac{1}{1-x}$$

$$\int_0^x \frac{(1+\varepsilon x)^2}{(1-x)^2}\,dx = 2\varepsilon(1+\varepsilon)\ln(1-x) + \varepsilon^2 x + \frac{(1+\varepsilon)^2 x}{1-x}$$

$$\int_0^x \frac{dx}{(1-x)(\Theta_B - x)} = \frac{1}{\Theta_B - 1}\ln\frac{\Theta_B - x}{\Theta_B(1-x)} \qquad \Theta_B \neq 1$$

°F = 1.8 × °C + 32
°R = °F + 459.69
K = °C + 273.16
R = 1.8 × K
°Réamur = 1.25 × °C