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UNIVERSITI TUN HUSSEIN ONN MALAYSIA

FINAL EXAMINATION
SEMESTER II
SESSION 2013/2014

COURSE NAME	:	CHEMICAL REACTION ENGINEERING
COURSE CODE	:	BNQ 20703
PROGRAMME	:	2 BNN
TEST DATE	:	JUNE 2014
DURATION	:	3 HOURS
INSTRUCTION	:	ANSWER **FOUR (4)** QUESTIONS ONLY

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

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Q1 The reaction is carried out isothermally in continuous-flow reactor.

$$A \rightarrow B$$

(a) Calculate the CSTR and PFR reactor volumes necessary to consume 99% of A, when the entering molar flow rate is 5mol/hr, entering volumetric is 10 dm^3/hr ($\upsilon = \upsilon_o$) and the reaction rate is :

(i) $-r_A = kC_A$, with k = 0.0001/s (10 marks)

(ii) $-r_A = kC_A^2$, with k = 3 dm^3/ mol.h (10 marks)

(b) If the reaction is changed and carried out in a 20 dm^3 batch reactor, calculate the time necessary to reduce the number of moles A in the reactor from 20 mol (initial mol) to 0.2 mol. The reaction rate is :

$$-r_A = kC_A \quad \text{with } \{k\} = 0.865/\text{min}$$

(5 marks)

Q2 Consider the gas-phase reaction below;

$$2SO_2 + O_2 \rightarrow 2SO_3$$

A mixture of 28% SO_2 and 72% air is charged in which SO_2 is oxidized. The reaction is carried out isothermally at temperature 227°C in a flow reactor with the total pressure of 1485kPa (neglect the pressure drop in the reaction).

(a) Construct stoichiometric table for the reaction using the symbol (i.e., Θ, F) with SO_2 as your basis of calculation.

(8 marks)

(b) Identify the entering concentration of SO_2 and the total concentration (C_T)

(5 marks)

(c) Identify the concentration of each species at 25% conversion..

(12marks)

Q3 The following complex liquid phase reaction is carried out in a 50L CSTR :

$$2A \xrightarrow{k1} 2B + C \qquad ; -r_{1A} = k_1 C_A^{\ 2}$$
$$A + 2C \xrightarrow{k2} D \qquad ; -r_{2C} = k_2 C_A C_C$$

100 mol/L of A is fed into the reactor at a constant rate of 20 L/min. The value of specific constants k_1 and k_2 are 0.35 (L/mol.min) and 0.25 (L/mol.min) respectively.

(a) Give the net rate of reaction for A, B, C and D.

(14 marks)

(b) Using the appropriate design equation, calculate the yield of C (Y_C) and selectivity of C over D (S_{CD}) that can be achieved after 90% of A consumed.

(5 marks)

(c) Explain on how would you design the system to get maximum product of C.

(6 marks)

Q4 The following exothermic reaction was carried out adiabatically and the following data recorded in Table 1 : $A \rightarrow B + C$

Table 1

X	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8
$-r_A$ (mol/dm^3.s)	0.0053	0.0052	0.0050	0.0045	0.0040	0.0033	0.0025	0.0018	0.00125

(a) Calculate the volume necessary to achieve 80% conversion (X = 0.8) when the entering conditions are υ_o = 6 dm^3/s, P_o = 10 atm, y_{Ao} =0.5, T_o = 422.2K . for reactor:

(i) CSTR

(ii) PFR

(15 marks)

(b) Draw the graph with shaded area of both reactor volume.

(5 marks)

(c) Select the effective/efficient reactor in terms of reactor volume.

(5 marks)

Q5 Methyl ethyl ketone (MEK) is an important industrial solvent that can be produced from the dehydrogenation of Butan-2-ol (Bu) over a zinc oxide catalyst.

$$Bu \rightarrow MEK + H_2$$

The following data giving the reaction rate for MEK were obtained in a differential reactor at 490°C.

P_{Bu} (atm)	**2**	**0.1**	**0.5**	**1**	**2**	**1**
P_{MEK} (atm)	5	0	2	1	0	0
P_{H2} (atm)	0	0	1	1	0	10
r'_{MEK} (mol/h.g cat.)	0.044	0.040	0.069	0.060	0.043	0.059

(a) Develop the rate law based on the experimental data.

(12 marks)

(b) Analyze a reaction mechanism and rate limiting step based on the rate law. (Some species might be weakly adsorbed).

(13 marks)

- END OF QUESTION -

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$F_{B0} = F_{A0}\Theta_B - \frac{b}{a}(F_{A0}X)$$

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

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

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

$$PV = ZR_T T$$

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

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

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

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

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

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

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

$$r_A = r_D + r_U$$

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

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

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

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

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

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

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

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