Universiti Tun Hussein Onn Malaysia

UNIVERSITI TUN HUSSEIN ONN MALAYSIA

FINAL EXAMINATION
SEMESTER II
SESSION 2015/2016

COURSE NAME	:	CHEMICAL REACTION ENGINEERING
COURSE CODE	:	BNQ 20304
PROGRAMME CODE	:	BNN
EXAMINATION DATE	:	JUNE / JULY 2016
DURATION	:	3 HOURS
INSTRUCTION	:	ANSWER **FOUR (4)** QUESTIONS ONLY

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

Q1 The elementary gas phase reaction with first order reaction is carried out in a plug flow reactor (PFR) with no pressure drop in which the volumetric flow rate is, υ, is constant.

$$A \rightarrow B$$

(a) List the assumption made in the derivation of the design equation for PFR.

(2 marks)

(b) Describe the changes of concentrations of the reactants and products with respect to time for the reaction carried out in a plug flow reactor.

(4 marks)

(c) Derive an equation relating the reactor volume to the entering and exiting concentration of A, the rate constant k, and the volumetric flow rate, υ.

(8 marks)

(d) Determine the reactor volume to reduce the exiting concentration to 10% of the entering concentration when the volumetric flow rate is 10 dm^3/min and rate constant, k, is 0.23 /min.

(3 marks)

(e) Calculate the reactor volumes if the reaction consume 99% of A at the entering molar flow rate is 5 mol/h. The reaction is a second order reaction and the reaction rate, k, is 3 dm^3/mol.min.

(8 marks)

Q2 In the hippopotamus, digestion occurs as an autocatalytic reaction in the stomach followed by a catalytic reaction in the intestines. This system can be modeled as a series of CSTR-PFR. The volumetric flow rate of food intake into the system can be assumed to be 100 L/d, at a concentration of 7.5 mol/L. The volume of the stomach (modeled as CSTR) is 450 L. Reciprocal rates (in mol/L-d) for the two types of reactions are provided in Table Q2 (i) and Table Q2 (ii):

Table Q2 (i): Autocatalytic reaction in the stomach

X	**0**	**0.1**	**0.2**	**0.3**	**0.4**	**0.5**	**0.6**	**0.7**	**0.8**
$1/-r_A$ (mol/L.d)	8.0	5.0	1.5	2.0	2.5	3.5	5.0	7.0	9.0

Table Q2 (ii): Catalytic reaction in the intensities

X	**0**	**0.1**	**0.2**	**0.3**	**0.4**	**0.5**	**0.6**	**0.7**	**0.8**
$1/-r_A$ (mol/L.d)	8.0	5.0	1.5	2.0	2.5	3.5	5.0	7.0	9.0

(a) Calculate the volume of the intestines if the total conversion of 50% is observed.

(15 marks)

(b) (i) Plot a graph which can indicate the volume of the intestines.
(ii) Shaded the area represent the volume in the graph.

(10 marks)

Q3 The isothermal reaction of nitric oxide produced by the gas phase oxidation of ammonia in a flow reactor is shown by the following reaction.

$$4NH_3 + 5O_2 \rightarrow 4NO + 6H_2O$$

The feed consists of 15 mol % ammonia in air at 8.2 atm and 227°C.

(a) Calculate the total entering concentration.

(3 marks)

(b) Determine the entering concentration of ammonia.

(2 marks)

(c) Develop a stoichiometric table for the reaction with ammonia as your basis of calculation.

(10 marks)

(d) Evaluate the concentration for each species involve in the reaction in terms of conversion.

(10 marks)

Q4 Consider the following reaction to produce 300 million pounds of ethylene a year from a feed stream of pure ethane in plug flow reactor.

$$C_2H_6 \longrightarrow C_2H_4 + H_2$$

The reaction is irreversible and follows an elementary rate law. We want to achieve 80% conversion of ethane, operating the reactor isothermally at 1100K at a pressure of 6atm. Assume that the reaction is first order with $k = 0.072 s^{-1}$ at 1000K.

(a) Express the concentration of each species in terms of conversion.

(6 marks)

(b) Calculate the entering concentration of species A.

(3 marks)

(c) Determine the volume at 80% conversion.

(7 marks)

(d) Examine the possible conversion that would achieved if the reaction occur in two $600 dm^3$ CSTR arranged in parallel reactor with entering volumetric fed to main stream is $10 dm^3$ with $k = 0.044 min^{-1}$.

(9 marks)

Q5 The following complex liquid phase reaction is carried out in a 50 L CSTR :

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

The concentration of A fed into the reactor is 100 mol/L. The flow rate into the reactor is constant and at 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) Carry out the net rate of reaction for A, B, C and D.

(14 marks)

(b) Using the appropriate design equation, calculate:

(i) the yield of C (Y_C)

(ii) the selectivity of C over D (S_{CD}) that can be achieved after 90% A is consumed.

(5 marks)

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

(6 marks)

- **END OF QUESTIONS** -

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

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

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

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

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

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

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

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

$$F_{A0} = C_{A0} v_0$$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\nu = \nu_0(1 + y_{A0}\delta X)\frac{P_0}{P}\frac{T}{T_0}$$

$$= \nu_0(1 + \varepsilon X)\frac{P_0}{P}\frac{T}{T_0}$$

$$PV = ZR_T T$$

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

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

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

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

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

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

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

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

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

$$r_A = r_D + r_U$$

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

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

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

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

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

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

R = 8.314 kPa.dm^3/molK

R = 1.987 cal/mol.K

0.73ft^3.atm/lbmol.°R

K = C +273.16

R = 1.8 × KR =

E = 82,000 cal/gmol