UNIVERSITY OF TECHNOLOGY, JAMAICA

COLLEGE/ FACULTY: Faculty of Engineering and Computing

SCHOOL/ DEPARTMENT: Engineering/ Chemical Engineering

Final Examination, Semester 1

Module Name:	**Chemical Reaction Engineering**
Module Code:	**CHE 3006**
Date: December	**2010**
Theory/ Practical:	**Theory**
Groups:	**Beng3C**
Duration:	**2 Hours**

Instructions

1. ANSWER ALL QUESTIONS

2. EACH QUESTION MUST BEGIN ON A NEW PAGE

3. LEAVE TWO LINES BETWEEN PARTS OF A QUESTION

4. SHOW CLEARLY ALL EQUATIONS USED FOR CALCULATIONS

5. ANSWER MUST BE NUMBERED IDENTICAL TO THE QUESTION BEING ANSWERED

6. THE INTENDED MARK IS INDICATED AT THE BEGINNING OF EACH QUESTION

7. FORMULA AND UNIT CONVERSION SHEETS ARE ATTACHED

DO NOT TURN PAGE UNTIL YOU ARE TOLD TO DO SO

Question 1:(10 marks)

The exothermic reaction $A \longrightarrow B + C$ was carried out adiabatically and the following data recorded:

X	0	0.2	0.4	0.45	0.5	0.6	0.8	0.9
$-r_A$ (mol/dm^3.min)	1.0	1.67	5.0	5.0	5.0	5.0	1.25	0.91

The entering molar flow rate of A was 300 mol/min.

a) What are the PFR and CSTR volumes necessary to achieve 40% conversion

[5]

b) Over what range of conversions would the CSTR and PFR reactor volumes be identical

[1]

c) Show graphically the volume of a PFR for 40% conversion followed by a CSTR for up to 80% conversion
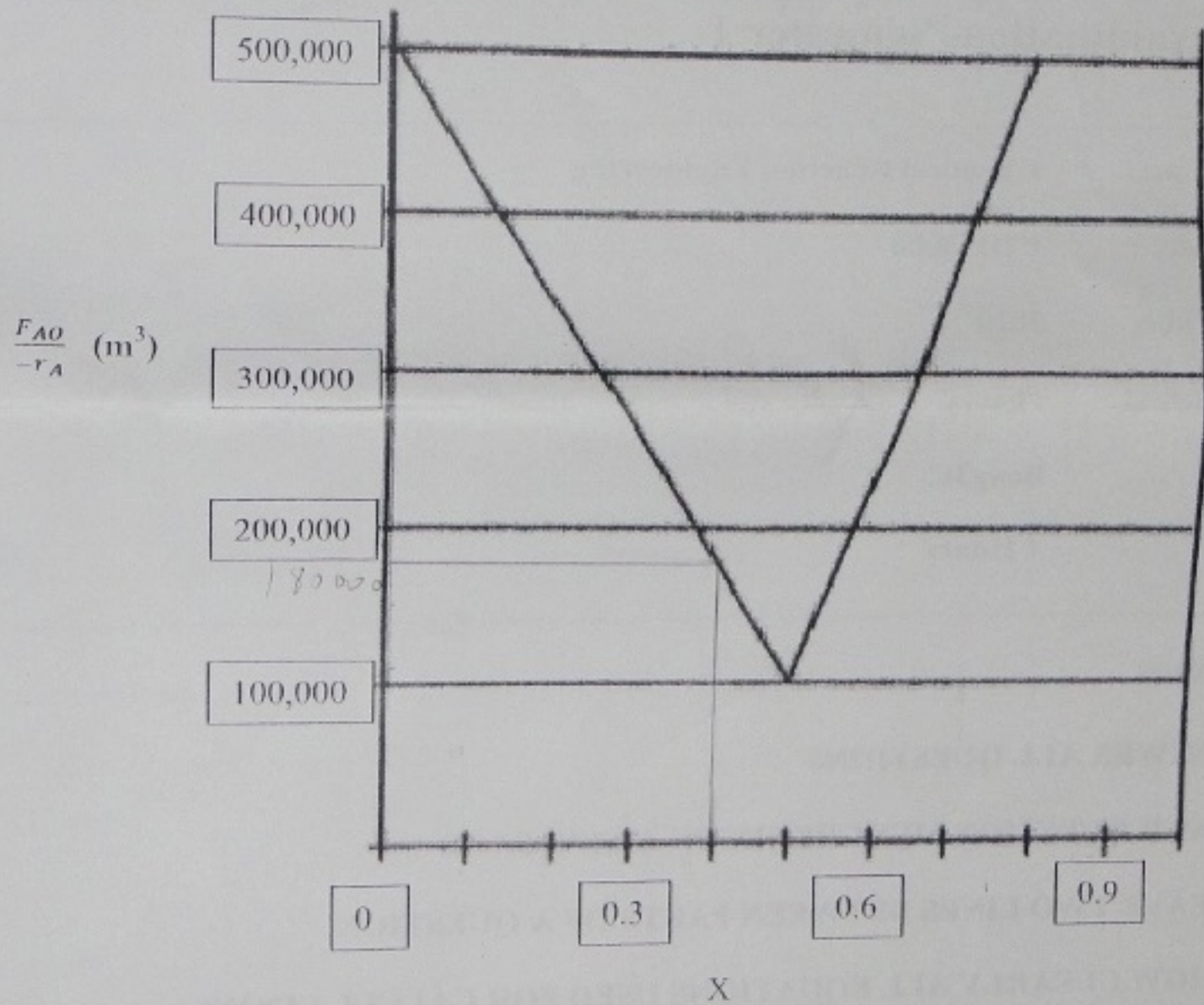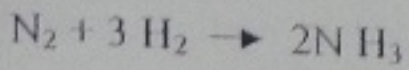
[1]

Figure 1. Levenspiel plot

d) Using Figure 1, what PFR volume is necessary to achieve 50% conversion and what CSTR volume is necessary to achieve 50% conversion?

[2]

e) Show the answers from part (d) graphically.

[1]

Question 2: (16 marks)

The gas phase reaction:

$$N_2 + 3H_2 \rightarrow 2NH_3$$

is to be carried out isothermally in a flow system with no pressure drops. The molar feed is 60% H_2 and 40% N_2 at a pressure of 15 atm and 200 °C.

a) Construct a stoichiometric table including a column for concentration

b) What are the values for C_{AO}, θ_B, θ_C, δ, and ε? [6]

c) Prove that Hydrogen is the limiting reactant [5]

d) Calculate the concentration of Nitrogen and ammonia at 55% conversion? [1]

e) Write a rate law in terms of conversion if it was second order in H_2 and overall first order. [2]

[2]

Question 3: (10 marks)

The gaseous reaction A $\rightarrow$ B has a unimolecular reaction rate constant of $0.0015\ min^{-1}$ at 80°F. This reaction is to be carried out in *parallel tubes* 3m long and 2.5cm inside diameter under a pressure of 1000kPa at 126°C. A production rate of 1000 g/h of B is required. Assuming an activation energy of 25,000 cal/mol, how many tubes are needed if the conversion of A is to be 90%? Assume perfect gas laws. A and B each have molecular weight of 58 g/mol.

$$1dm^3 = 1000cm^3$$

$$PV = nRT$$

$$V = \frac{nRT}{P}$$

In order to study the photochemical decay of aqueous bromine in bright sunlight, a small quantity of liquid bromine was dissolved in water contained in a glass battery jar and placed in direct sunlight. The following data were obtained:

Temperature = $25°C$

Time (min)	10	20	30	40	50	60
Ppm Br_2	2.45	1.74	1.23	0.88	0.62	0.44

a) Determine whether the reaction rate is zero, first, or second order in bromine, and calculate the reaction rate constant in units of your choice.

[10]

b) Assuming identical exposure conditions, calculate the required hourly rate of injection of bromine (in grams) into a sunlit body of water, 25,000 gal in volume, in order to maintain a sterilizing level of bromine of 1.0 ppm

[4]

ppm= mg/l   1gal=3.785L

TOTAL MARKS = 50

END OF EXAM

1 Useful Integrals in Reactor Design

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

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

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

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

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

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

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

2. *Simpson's one-third rule* (three-point)   A more accurate evaluation of the integral can be found with the application of Simpson's rule:

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

where

$$h = \frac{X_2 - X_0}{2} \qquad X_1 = X_0 + h$$

Ideal Gas Constant

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

$$R = \frac{8.314 \text{ kPa} \cdot \text{dm}^3}{\text{mol} \cdot K}$$

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

$$R = \frac{1.987 \text{ Btu}}{\text{lb-mol} \cdot {}^\circ R}$$

$$R = \frac{8.3144 \text{ J}}{\text{mol} \cdot K}$$

$$R = \frac{1.987 \text{cal}}{\text{mol} \cdot K}$$

Boltzmann's constant $k_B = 1.381 \times 10^{-23} \dfrac{J}{\text{molecule} \cdot K}$

$$= 1.381 \times 10^{-23} \text{ kg m}^2/\text{s}^2/\text{molecule}/K$$

Volume of Ideal Gas

1 lb-mol of an ideal gas at 32°F and 1 atm occupies 359 ft³ (0.00279 lbmol/ft³).
1 mol of an ideal gas at 0°C and 1 atm occupies 22.4 dm³ (0.0446 mol/dm³).

$$C_A = \frac{P_A}{RT} = \frac{y_A P}{RT}$$

where C_A = concentration of A, mol/dm³ T = temperature, K
P = pressure, kPa y_A = mole fraction of A
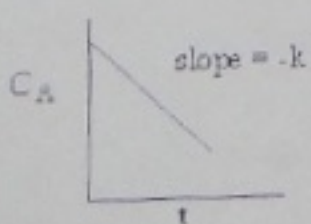R = ideal gas constant, 8.314 kPa·dm³/mol·K

Appendix

Reactor	Differential	Algebraic	Integral	Differential	Algebraic	Integral
Batch	$\dfrac{dN_A}{dt} = r_A V$		$t = \displaystyle\int_{N_{A0}}^{N_A} \dfrac{dN_A}{r_A V}$	$N_{A0}\dfrac{dX}{dt} = -r_A V$		$t = N_{A0}\displaystyle\int_0^X \dfrac{dX}{-r_A V}$
CSTR		$V = \dfrac{F_{A0} - F_A}{-r_A}$			$V = \dfrac{F_{A0}X}{-r_A}$	
PFR	$\dfrac{dF_A}{dV} = r_A$		$V = \displaystyle\int_{F_{A0}}^{F_A} \dfrac{dF_A}{r_A}$	$F_{A0}\dfrac{dX}{dV} = -r_A$		$V = F_{A0}\displaystyle\int_0^X \dfrac{dX}{-r_A}$
PBR	$\dfrac{dF_A}{dW} = r_A'$		$W = \displaystyle\int_{F_{A0}}^{F_A} \dfrac{dF_A}{r_A'}$	$F_{A0}\dfrac{dX}{dW} = -r_A'$		$W = F_{A0}\displaystyle\int_0^X \dfrac{dX}{-r_A}$

$$k = Ae^{-E/RT}$$

$$k(T_2) = k(T_1)\exp\left[\frac{E}{R}\left(\frac{1}{T_1} - \frac{1}{T_2}\right)\right]$$

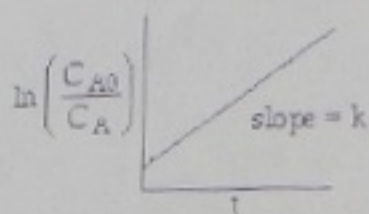| Zero Order	First Order	Second Order
Zero order. $\alpha = 0$	First order $\alpha = 1$	Second order $\alpha = 2$

$$\frac{dC_A}{dt} = r_A = -k \qquad \frac{dC_A}{dt} = r_A = -kC_A \qquad \frac{dC_A}{dt} = r_A = -kC_A^2$$

at $t = 0$, $C_A = C_{A0}$ at $t = 0$, $C_A = C_{A0}$ at $t = 0$, $C_A = C_{A0}$

$$\Rightarrow C_A = C_{A0} - kt \qquad \Rightarrow \ln\left(\frac{C_{A0}}{C_A}\right) = kt \qquad \Rightarrow \frac{1}{C_A} - \frac{1}{C_{A0}} = kt$$