NATIONAL UNIVERSITY OF SCIENCE AND TECHNOLOGY

FACULTY OF INDUSTRIAL TECHNOLOGY
BACHELOR OF ENGINEERING (HONS) DEGREE
Part Two Examination May 2011

TCE 2008 Chemical Reaction Engineering I

Duration of Examination 3 Hours

Instructions to Candidates:
Answer ALL FIVE questions.
Each question carries equal marks.
Show all your steps clearly in your calculation.
Start the answers for each question on a new page.

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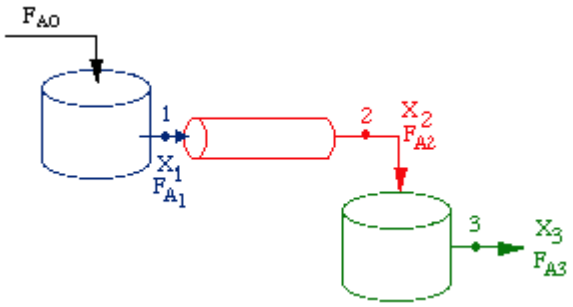
1. The isomerization of butane: $n-C_4H_{10} \Leftrightarrow i-C_4H_{10}$ was carried out adiabatically in the liquid-phase and the data were obtained:

X	0	0.2	0.4	0.6	0.65
$-r_A (mol/m^3 h)$	39	53	59	38	25

The reactor scheme:



Calculate the volume of each of the reactors for an entering molar flow rate of *n-butane* of *50 kmol/hr*. **[20] marks)**

2. Nitric acid is made commercially from nitric oxide. Nitric oxide is produced by the gas-phase oxidation of ammonia: $4NH_3 + 5O_2 \rightarrow 4NO + 6H_2O$

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

a) What is the total entering concentration? **[2]**

b) What is the entering concentration of ammonia? **[3]**

c) Set up a stoichiometric table with ammonia as your basis of calculation.

i. Express Ci for all species as functions of conversion for a constant-volume batch reactor. **[5]**

ii. Express Pi and Ci for all species as functions of conversion for a flow reactor. **[5]**

d) Write the combined mole balance and rate law solely in terms of the molar flow rates and rate law parameters for C_1 and C_2 above. Assume the reaction is first order in both reactants **[5]**

3. Dibutyl phthalate (DBP), a plasticizer, has a potential market of 12 million lb/year and is to be produced by reaction of *n-butanol* with *monobutyl phthalate* (MBP).

$$MBP + n - buta.nol \xrightarrow{H_2SO_4} DBP + H_2O$$

The reaction follows an elementary rate law and it catalyzed by H_2SO_4. A stream containing MBP and butanol is to be mixed with the H_2SO_4 catalyst immediately before the stream enters the reactor. The concentration of MBP in the stream entering the reactor is 0.2 lb-mol/ft^3, and the molar feed rate of butanol is five times that of MBP. The specific reaction rate at 100°F is 1.2 ft^3/mol-lb h. There is a 1000 US gallon CSTR and associated peripheral equipment available for use on this project for 30 days a year (oparating 24 *h/day*).

a) Determine the exit conversion in the available 1000 gallon reactor if you were to produce 33% of the share of the predicted market. **[10]**

b) For the same temperature, what CSTR volume would be necessary to achieve a conversion of 85% for a molar feed rate of MBP of 1 lb-mol/min? **[5]**

c) Calculate the tubular reactor volume necessary to achieve 85% conversion. **[5]**

4. Determine the reaction order for the gas-phase decomposition of di-tert-butyl peroxide:

$$(CH_3)_3COOC(CH_3)_3 \rightarrow C_2H_6 + 2CH_3CH_3$$

This reaction was carried out in the laboratory in an isothermal batch system in which the total pressure was recorded at various times during the reaction. The data given in Table 1.

Only pure di-tert-butyl peroxide was initially present in the reaction vessel.

Time (min)	0	2.5	5.0	10	15	20
Total Pressure(*mmHg*)	7.5	10.5	12.5	15.8	17.9	19.4

Table 1.

Use graphical method to determine reaction order

[20]

5. The irreversible elementary gas phase reaction 2A →B+C is currently carried out in a packed bed reactor containing 100 kg of catalyst. The entering pressure is 20 atm and the exit pressure is 4 atm. Currently 50% conversion is achieved. It is proposed to add a CSTR with 200 kg of catalyst downstream of the PBR. The is no pressure drop in the CSTR. The flow rate and temperature remain unchanged.

a) What would be the overall conversion in such an arrangement? **[15]**

b) Is there better way to carry out the reaction, and if so what is it? **[5]**