UNIVERSITI TEKNOLOGI PETRONAS

FINAL EXAMINATION
MAY 2024 SEMESTER

COURSE	:	**CEB2043/CFB2053 - REACTION ENGINEERING I**
DATE	:	**12 AUGUST 2024 (MONDAY)**
TIME	:	**9.00 AM - 12.00 NOON (3 HOURS)**

INSTRUCTIONS TO CANDIDATES

1. Answer **ALL** questions in the Answer Booklet.

2. Begin **EACH** answer on a new page in the Answer Booklet.

3. Indicate clearly answers that are cancelled, if any.

4. Where applicable, show clearly steps taken in arriving at the solutions and indicate **ALL** assumptions, if any.

5. **DO NOT** open this Question Booklet until instructed.

Note :

i. There are **SEVEN (7)** pages in this Question Booklet including the cover page and appendix.

ii. **DOUBLE-SIDED** Question Booklet.

iii. **Graph paper will be provided.**

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1. a. Explain the importance of Chemical Reaction Engineering knowledge to a chemical engineer.

   [6 marks]

   b. Liquid phase isomerization of xylenes was carried out adiabatically at 250°C. The reaction rate data is summarized in **TABLE Q1**. The reactant enters the reactor at 50 kmol/h with initial concentration of 4 mol/dm^3.

   TABLE Q1: Conversion, X, versus. reaction rate, $-r_A$, data

X	0.0	0.2	0.3	0.4	0.6	0.7	0.9
$-r_A$ (mol/dm^3·s)	0.050	0.030	0.025	0.020	0.011	0.008	0.005

   i. With the help of Levenspiel Plot, determine the best flow reactor to convert 80% of the reactant. Justify your answer.

   [15 marks]

   ii. Calculate the space time, τ, for the proposed reactor in **part (b)(i)**.

   [5 marks]

2. An elementary gas phase reaction $A \rightarrow B + 2C$ is carried out in a flow reactor under isothermal condition with negligible pressure drop. The reaction rate constant, k, at 127°C is 0.001 min^{-1}. Pure reactant A flows at 10 atm and 127°C with entering molar flow rate of 2.5 mol/min.
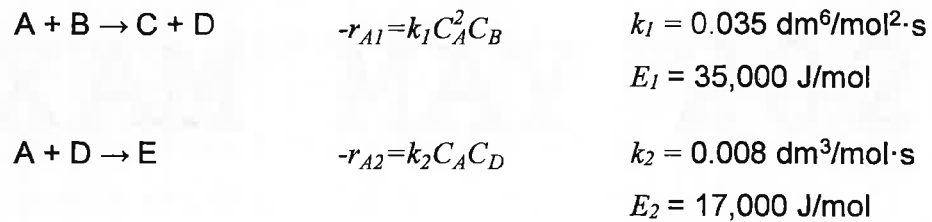
   a. Identify the best flow reactor (CSTR or PFR) to achieve 80% conversion of reactant A. State **THREE (3)** appropriate assumptions made in your calculation. Justify your answer.

   [20 marks]

   b. Evaluate the effect of neglecting the expansion factor in designing the reactor in **part (a)**.
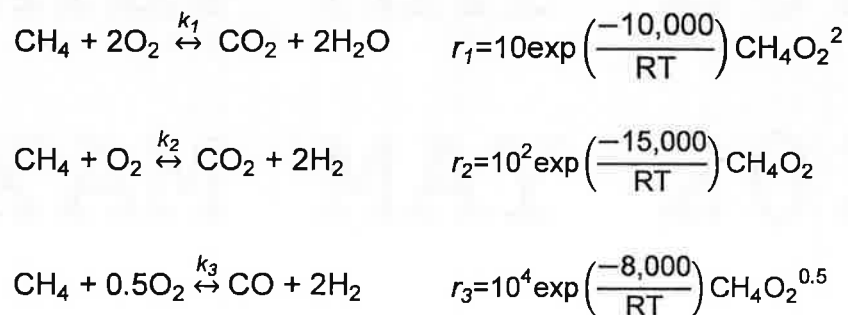
   [4 marks]

3. a. Gas product, D, is produced from multiple reactions involving two reactants, A and B, as per the following chemical reactions scheme and reaction kinetics:

$A + B \rightarrow C + D$ $-r_{A1}=k_1 C_A^2 C_B$ $k_1 = 0.035$ dm^6/mol$^2 \cdot$s

$E_1 = 35,000$ J/mol

$A + D \rightarrow E$ $-r_{A2}=k_2 C_A C_D$ $k_2 = 0.008$ dm^3/mol$\cdot$s

$E_2 = 17,000$ J/mol

Propose the best reactor scheme and operating conditions (concentration and temperature) to maximize the desired product and minimize the byproduct. Justify your proposal with appropriate diagram.

[12 marks]

b. Methane (CH_4) is partially oxidized in auto thermal reforming process to produce the desired product, carbon monoxide (CO) and hydrogen (H_2) gas. At the same time, the by-product CO_2 and H_2O are also produced in the following multiple reactions:

$CH_4 + 2O_2 \overset{k_1}{\leftrightarrow} CO_2 + 2H_2O$ $r_1=10\exp\left(\dfrac{-10,000}{RT}\right)CH_4 O_2^2$

$CH_4 + O_2 \overset{k_2}{\leftrightarrow} CO_2 + 2H_2$ $r_2=10^2\exp\left(\dfrac{-15,000}{RT}\right)CH_4 O_2$

$CH_4 + 0.5O_2 \overset{k_3}{\leftrightarrow} CO + 2H_2$ $r_3=10^4\exp\left(\dfrac{-8,000}{RT}\right)CH_4 O_2^{0.5}$

This process is to be conducted in PFR. Identify suitable reactor scheme and operating conditions (concentration and temperature) to maximize the desired product. Justify your answer with appropriate illustration.

[14 marks]

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4. The isomerization of normal pentane (n-C_5H_{12}) to produce isopentane (i-C_5H_{12}) is conducted adiabatically in a flow reactor by following the elementary reaction below:
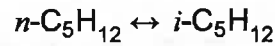
$$n\text{-}C_5H_{12} \leftrightarrow i\text{-}C_5H_{12}$$

The total molar flowrate entering the reactor is 120 kmol/h at 150°C with 70 mol% of n-C_5H_{12} and the balance is inert gas.

Given that:

- ΔH_{RX} = 25.14 kJ/mol
- Activation energy, E = 23.7 kJ/mol
- k = 22.3 h^{-1} at 360 K
- K_c = 2.05 at 333 K
- $C_{p,n\text{-}C_5H_{12}}$ = 225 J/mol·K at 273 K
- $C_{p,i\text{-}C_5H_{12}}$ = 225 J/mol·K at 273 K
- $C_{p,inert}$ = 350 J/mol·K at 273 K

Evaluate the possibility to achieve 80% conversion for this process. Justify your answer with appropriate calculations.

[24 marks]

- END OF PAPER –

APPENDIX

Numerical Integration of Integrals:

1. Trapezoidal rules

$$\int_{X_0}^{X_1} f(X)dX = \frac{h}{2}[f(X_0) + f(X_1)] \qquad where \quad h = X_1 - X_0$$

2. Simpson's one-third rules (three points)

$$\int_{X_0}^{X_2} f(X)dX = \frac{h}{3}[f(X_0) + 4f(X_1) + f(X_2)] \qquad where \quad h = \frac{X_2 - X_0}{2}$$

3. Simpson's three-eight rules (four points)

$$\int_{X_0}^{X_3} f(X)dX = \frac{3}{8}h[f(X_0) + 3f(X_1) + 3f(X_2) + f(X_3)]$$

$$where \quad h = \frac{X_3 - X_0}{3}$$

4. Five points quadrature formula

$$\int_{X_0}^{X_4} f(X)dX = \frac{h}{3}[f(X_0) + 4f(X_1) + 2f(X_2) + 4f(X_3) + f(X_4)]$$

$$where \quad h = \frac{X_4 - X_0}{4}$$

Useful integrals in reactor design:

$$\int_0^X \frac{dX}{X^2} = -\frac{1}{X}$$

$$\int_0^X \frac{dX}{1 - X} = \ln\frac{1}{1 - X}$$

$$\int_0^X \frac{dX}{(1 - X)^2} = \frac{X}{1 - X}$$

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$$\int_0^X \frac{dX}{(1 + \varepsilon X)} = \frac{1}{\varepsilon} \ln (1 + \varepsilon X)$$

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

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

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

$$\int_0^X \frac{dX}{(1 - X)(M - X)} = \frac{1}{M - 1} \ln \frac{M - X}{M(1 - X)} \qquad M \neq 1$$

General equation for non-isothermal reactor energy balance:

$$\dot{Q} - \dot{W}_s - F_{A0} \sum \theta_i C_{Pi}(T - T_0) - F_{A0}X[\Delta H_{RX}^0(T_R) + \Delta C_P(T - T_R)] = 0$$

Other useful information:

- Arrhenius relationship

$$k_{2(T)} = k_{1(T_1)} exp \left[\frac{E}{R} \left(\frac{1}{T_1} - \frac{1}{T} \right) \right]$$

$$K_{C(T)} = K_{C(T_2)} exp \left[\frac{\Delta H_{RX}^0}{R} \left(\frac{1}{T_2} - \frac{1}{T} \right) \right]$$

- Ideal gas constant:

  R = 8.314 kPa·dm³·mol⁻¹·K⁻¹

  = 8.314 J·mol⁻¹·K⁻¹

  = 0.082 dm³·atm·mol⁻¹·K⁻¹

  = 0.082 m³·atm·kmol⁻¹·K⁻¹

- Energy conversion:

  1 cal = 4.18 J

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