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UNIVERSITI SAINS MALAYSIA

First Semester Examination  
Academic Session 2008/2009

November 2008

**EKC 336 – Chemical Reaction Engineering**  
***[Kejuruteraan Tindakbalas Kimia]***

Duration : 3 hours  
*[Masa : 3 jam]*

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Please check that this examination paper consists of SIX pages of printed material and TWO pages of Appendix before you begin the examination.

*[Sila pastikan bahawa kertas peperiksaan ini mengandungi ENAM muka surat yang bercetak dan DUA muka surat Lampiran sebelum anda memulakan peperiksaan ini.]*

**Instructions:** Answer any **FOUR** (4) questions.

**Arahan:** Jawab mana-mana **EMPAT** (4) soalan.]

You may answer a question either in Bahasa Malaysia or in English.

*[Anda dibenarkan menjawab soalan sama ada dalam Bahasa Malaysia atau Bahasa Inggeris.]*

Answer any FOUR questions.

Jawab mana-mana EMPAT soalan.

1. [a] The rate of hydration of ethylene oxide (A) to ethylene glycol ( $C_2H_4O + H_2O \rightarrow C_2H_6O_2$ ) in dilute aqueous solution is proportional to the concentration of A, with the proportionality constant  $k_A = 4.11 \times 10^{-5} \text{ s}^{-1}$  at  $20^\circ\text{C}$  for a certain catalyst. Determine the half-life ( $t_{1/2}$ ) for a batch reactor and space-time ( $\tau_{1/2}$ ) for a CSTR reactor operating at steady state of the oxide (A) at  $20^\circ\text{C}$

*Kadar penghidratan etilena oksida (A) kepada etilena glikol ( $C_2H_4O + H_2O \rightarrow C_2H_6O_2$ ) dalam larutan akueus cair adalah berkadar langsung dengan kepekatan A dan pemalar kadaran  $k_A = 4.11 \times 10^{-5} \text{ s}^{-1}$  pada  $20^\circ\text{C}$  untuk sejenis mangkin tertentu. Tentukan separuh-hayat ( $t_{1/2}$ ) untuk sebuah reaktor kelompok dan masa ruang ( $\tau_{1/2}$ ) untuk sebuah reaktor CSTR yang beroperasi pada keadaan mantap bagi oksida (A) pada  $20^\circ\text{C}$*

[6 marks/markah]

- [b] An aqueous solution of ethyl acetate (A), with a concentration of  $0.30 \text{ mol L}^{-1}$  and flowing at  $0.50 \text{ L s}^{-1}$ , mixes with an aqueous solution of sodium hydroxide (B), of concentration  $0.45 \text{ mol L}^{-1}$  and flowing at  $1.0 \text{ L s}^{-1}$ . The combined stream enters a CSTR of volume  $500 \text{ L}$ . If the reactor operates at steady-state, and the fractional conversion of ethyl acetate in the exit stream is  $0.807$ , what is the rate of reaction ( $-r_A$ )?

*Suatu larutan akueus etil asetat (A), dengan kepekatan  $0.30 \text{ mol L}^{-1}$  mengalir pada  $0.50 \text{ L s}^{-1}$ , dan bercampur dengan suatu larutan akueus sodium hidroksida (B), yang berkepekatan  $0.45 \text{ mol L}^{-1}$  dan mengalir pada  $1.0 \text{ L s}^{-1}$ . Aliran tergabung tersebut memasuki sebuah CSTR yang berisipadu  $500 \text{ L}$ . Jika reaktor tersebut beroperasi pada keadaan mantap dan penukaran pecahan etil asetat dalam aliran keluar ialah  $0.807$ , apakah kadar tindakbalas ( $-r_A$ )?*

[8 marks/markah]

- [c] A homogeneous gas reaction  $A \rightarrow 3B$  has a reported rate at  $215^\circ\text{C}$  as

$$-r_A = 0.01 C_A^{1/2}, \quad [\text{mol/L.S}]$$

Find the space-time needed for  $80\%$  conversion of A in a feed containing  $50\%$  A and  $50\%$  inert feed to a plug flow reactor operating at  $215^\circ\text{C}$  and  $5 \text{ atm}$ . The initial concentration of A is  $0.0625 \text{ mol/L}$ :

*Suatu tindakbalas gas homogen  $A \rightarrow 3B$  telah dilaporkan mempunyai kadar pada  $215^\circ\text{C}$*

$$-r_A = 0.01 C_A^{1/2}, \quad [\text{mol/L.S}]$$

*Carikan masa ruang yang diperlukan bagi penukaran  $80\%$  A untuk reaktor aliran palam yang beroperasi pada  $215^\circ\text{C}$  dan  $5 \text{ atm}$  dengan suatu suapan yang mengandungi  $50\%$  A dan  $50\%$  bahan lengai. Kepekatan awal A ialah  $0.0625 \text{ mol/L}$ .*

[8 marks/markah]

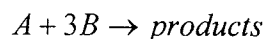
...3/-

- [d] In general what are the parameters affecting the rate of reaction?

*Secara umumnya, apakah parameter-parameter yang memberi kesan terhadap kadar tindakbalas?*

[3 marks/markah]

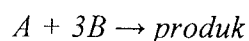
2. [a] The rate law for the reaction  $C_2H_4Br_2 + 3KI \rightarrow C_2H_4 + 2KBr + KI_3$  in an inert solvent, which can be written as



has been found to be  $(-r_A) = k_A C_A C_B$ , with the rate constant

$$k_A = 1.34 \text{ L mol}^{-1} \text{ h}^{-1} \text{ at } 749^\circ\text{C}$$

*Hukum kadar bagi tindakbalas  $C_2H_4Br_2 + 3KI \rightarrow C_2H_4 + 2KBr + KI_3$  dalam suatu larutan lengai yang boleh ditulis sebagai*



*telah ditemui sebagai  $(-r_A) = k_A C_A C_B$ , dengan pemalar kadar*

$$k_A = 1.34 \text{ L mol}^{-1} \text{ jam}^{-1} \text{ pada } 749^\circ\text{C}$$

- [i] For the rate of disappearance of KI,  $(-r_B)$ , what is the value of rate constant  $k_B$ ?

*Apakah nilai pemalar kadar  $k_B$  bagi kadar kehilangan KI,  $(-r_B)$ ?*

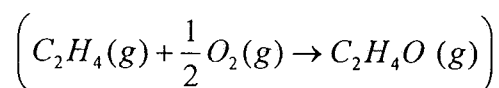
- [ii] At what rate KI being used when the concentrations are  $C_A = 0.022$  dan  $C_B = 0.22 \text{ mol L}^{-1}$ ?

*Apakah kadar penggunaan KI apabila kepekatan-kepekatan  $C_A = 0.022$  and  $C_B = 0.22 \text{ mol L}^{-1}$ ?*

[6 marks/markah]

- [b] For the gas phase oxidation of ethylene to ethylene oxide by the equation

*Untuk pengoksidaan fasa gas etilena kepada etilena oksida menurut persamaan*



- [i] Construct a stoichiometric table in terms of mole on the basis that only the reactants are present initially, and ethylene is the limiting reactant.

*Bina suatu jadual stoikiometri dalam ungkapan mol bagi asas-asas yang berikut; hanya bahan tindakbalas yang hadir di peringkat awal dan etilena ialah bahan tindakbalas menghad.*

- [ii] Repeat [i] in terms of concentration when  $O_2$  is the limiting reactant.

*Ulangi [i] dalam ungkapan kepekatan apabila  $O_2$  ialah bahan tindakbalas menghad.*

[10 marks/markah]

...4/-

[c] What are the main advantages and disadvantages of the following reactors:

*Apakah kelebihan-kelebihan dan kekurangan-kekurangan utama reaktor-reaktor yang berikut:*

- [i] Batch  
*Kelompok*
- [ii] Continuous stirred tank  
*Tangki teraduk berterusan*
- [iii] Plug flow  
*Aliran palam*

[9 marks/markah]

3. [a] The reaction ( $A \rightarrow B + C$ ) is carried out in a plug flow reactor. Determine the reaction order,  $\alpha$ , and the specific reaction rate constant ( $k$ ) by using the following data:

*Bagi tindakbalas ( $A \rightarrow B + C$ ) yang di jalankan dalam sebuah reaktor aliran palam, tentukan tertib tindakbalas,  $\alpha$ , dan pekali kadar tindakbalas tentu ( $k$ ) dengan menggunakan data yang berikut:*

time (hr) <i>masa (jam)</i>	0	5	10	15	20
$C_A$ (mol/L)	2.31	1.54	0.94	0.63	0.42

[9 marks/markah]

[b] Rate constants ( $k$ ) for the first order decomposition of nitrogen pentoxide at various temperatures are as follows:

*Pekali kadar ( $k$ ) untuk penguraian tertib pertama nitrogen pentoksida pada pelbagai suhu adalah seperti yang berikut:*

<b>T (K)</b>	273	298	308	318	328	338
$k$ ( $10^5 \text{ s}^{-1}$ )	0.0787	3.46	13.50	49.80	150	487

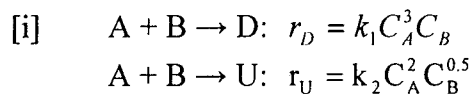
Calculate the activation energy and the pre-exponential factor for this reaction.

*Kirakan tenaga pengaktifan dan faktor pra-eksponen untuk tindakbalas ini.*

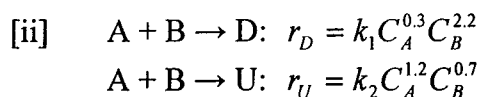
[4 marks/markah]

[c] Select the reactor schemes that will maximize the selectivity of the desired product,  $S_{D/U}$ , for the following parallel reactions:

*Pilih skema-skema reaktor yang akan memaksimumkan kememilihan produk yang dikehendaki,  $S_{D/U}$ , bagi tindakbalas-tindakbalas selari yang berikut:*



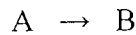
[6 marks/markah]



[6 marks/markah]

4. Component A is converted to B in a reactor.

*Komponen A ditukarkan kepada B dalam sebuah reaktor.*



The reaction is to be carried out adiabatically in the liquid phase under high pressure using trace amount of liquid catalyst which gives a specific reaction rate of  $31.1 \text{ h}^{-1}$  at 360 K. With the feed entering at 330 K, find the reactor volume necessary to process 163 kmol/h at 40% conversion of a mixture 90 mol % A and 10 mol % C, which is considered an inert.

*Tindakbalas tersebut dijalankan secara adiabatik dalam fasa cecair di bawah tekanan tinggi dengan menggunakan amaun pemangkin cecair yang sangat kecil, yang mana memberi kadar tindakbalas spesifik  $31.1 \text{ jam}^{-1}$  pada 360 K. Dengan suapan masuk pada suhu 330 K, carikan isipadu reaktor yang diperlukan untuk memproses 163 kmol/jam pada 40% penukaran bagi suatu campuran 90 mol % A dan 10 mol % C, yang dianggap suatu bahan lengai.*

- [i] Develop the design equation through mol balance, and energy balance in order to calculate the CSTR volume necessary to achieve 40% conversion for the above conditions.

*Bangunkan persamaan rekabentuk melaluiimbangan mol, danimbangan tenaga untuk mengira isipadu CSTR yang diperlukan untuk mencapai penukaran sebanyak 40% untuk keadaan di atas.*

[15 marks/markah]

- [ii] Find the equilibrium conversion for the reaction.

*Carikan penukaran keseimbangan bagi tindakbalas tersebut*

[4 marks/markah]

- [iii] If a PFR is used for the reaction at 40% conversion, discuss the volume needed comparing to that of a CSTR.

*Jika sebuah PFR digunakan untuk tindakbalas tersebut pada penukaran 40%, bincangkan isipadu reaktor PFR yang diperlukan berbanding dengan isipadu CSTR yang diperlukan.*

[6 marks/markah]

Additional information:

$$\Delta H_{Rx}^{\circ} = -6900 \text{ J/mol A ,}$$

$$\text{Activation energy} = 65.7 \text{ kJ/mol}$$

$$k_A/k_B = 3.03 \text{ at } 333 \text{ K}$$

$$C_{A_0} = 9.3 \text{ kmol/m}^3$$

Specific heat capacities:

$$C_{P_A} = C_{P_B} = 141 \text{ J/mol.K}$$

$$C_{P_C} = 161 \text{ J/mol.K}$$

Adiabatic energy balance:

$$X = \frac{\sum \Theta_i C_{P_i} (T - T_{i0})}{-[\Delta H_{Rx}^{\circ} (T_R) + \Delta C_P (T - T_R)]}$$

*Maklumat tambahan:*

$$\Delta H_{Rx}^{\circ} = -6900 \text{ J/mol A ,}$$

$$\text{Tenaga pengaktifan} = 65.7 \text{ kJ/mol}$$

$$k_A/k_B = 3.03 \text{ pada } 333 \text{ K}$$

$$C_{A_0} = 9.3 \text{ kmol/m}^3$$

...6/-

Haba muatan tentu:

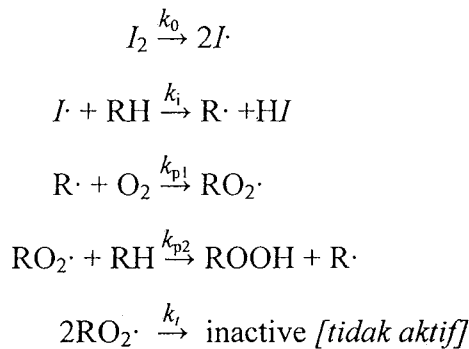
$$C_{p_A} = C_{p_B} = 141 \text{ J/mol.K}$$

$$C_{p_C} = 161 \text{ J/mol.K}$$

Imbangan tenaga adiabatik: 
$$X = \frac{\sum \Theta_i C_{p_i} (T - T_{i0})}{-\left[ \Delta H_{R_x}^o (T_R) + \Delta C_p (T - T_R) \right]}$$

5. [a] One of the major reasons for engine oil degradation is the oxidation. The suggested mechanism at low temperatures for the reaction is

*Salah satu sebab utama bagi penurunan minyak enjin ialah pengoksidaan. Mekanisme yang dicadangkan pada suhu rendah bagi tindakbalas tersebut ialah:-*



Where  $I_2$  is an initiator and RH is the hydrocarbon in the oil. Derive a rate law for the degradation of the engine oil.

*Di mana  $I_2$  sebagai pemula dan RH sebagai hidrokarbon dalam minyak. Terbitkan hukum kadar bagi penurunan minyak enjin.*

[10 marks/markah]

- [b] The feed flow through a reactor is  $10 \text{ dm}^3/\text{min}$ . A pulse test gave the following measurements at the outlet:

*Aliran suapan melalui sebuah reaktor adalah sebanyak  $10 \text{ dm}^3/\text{min}$ . Suatu ujian denyut memberi ukuran pada alur keluar yang seperti berikut:*

$t(\text{min})$	0	0.4	1.0	2	3	4	5
$C \times 10^3 \text{ g/dm}^3$	0	1	3	7.4	9.4	9.7	9.4
$t(\text{min})$	6	8	10	15	20	25	30
$C \times 10^3 \text{ g/dm}^3$	8.2	5.0	2.5	1.2	0.5	0.2	0

- [i] Plot the external age distribution  $E(t)$  curve as a function of time.  
*Plotkan lengkung agihan penuaan luar  $E(t)$  sebagai suatu fungsi masa.*
- [ii] Plot the internal age cumulative distribution  $F(t)$  curve as a function of time.  
*Plotkan lengkung agihan kumulatif penuaan dalam  $F(t)$  sebagai suatu fungsi masa.*

[15 marks/markah]

Appendix  
Lampiran

Numerical Evaluation of Integrals:

1. Trapezoidal rule

$$\int_{x_0}^{x_1} f(x) dx = \frac{h}{2} [f(x_0) + f(x_1)] \text{ when } h = x_1 - x_0$$

2. Simpson's three-eighths rule

$$\int_{x_0}^{x_3} f(x) dx = \frac{3}{8} h [f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)]$$

$$\text{Where } h = \frac{x_3 - x_0}{3}; \quad x_1 = x_0 + h; \quad x_2 = x_0 + 2h;$$

3. Simpson's quadrature formula

$$\int_{x_0}^{x_4} f(x) dx = \frac{h}{3} [f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + f(x_4)]$$

$$\text{Where } h = \frac{x_4 - x_0}{4}$$

4. For N+1 points, where (N/3) is an integer,

$$\int_{x_0}^{x_N} f(x) dx = \frac{3}{8} h [f(x_0) + 3f(x_1) + 3f(x_2) + 2f(x_3) + 3f(x_4) + 3f(x_5) + \dots + 3f(x_{N-1}) + f(x_N)]$$

$$\text{Where } h = \frac{x_N - x_0}{N}$$

5. For N+1 points, where N is even,

$$\int_{x_0}^{x_N} f(x) dx = \frac{h}{3} [f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \dots + 4f(x_{N-1}) + f(x_N)]$$

$$\text{Where } h = \frac{x_N - x_0}{N}$$

Ideal gas constant

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

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

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

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

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

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

## Useful Integrals in Reactor Design

$$\int_0^x \frac{dx}{1-x} = \ln \frac{1}{1-x} \quad (\text{A-1})$$

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

$$\int_0^x \frac{dx}{1+\varepsilon x} = \frac{1}{\varepsilon} \ln(1+\varepsilon x) \quad (\text{A-3})$$

$$\int_0^x \frac{1+\varepsilon x}{1-x} dx = (1+\varepsilon) \ln \frac{1}{1-x} - \varepsilon x \quad (\text{A-4})$$

$$\int_0^x \frac{1+\varepsilon x}{(1-x)^2} dx = \frac{(1-\varepsilon)x}{1-x} - \varepsilon \ln \frac{1}{1-x} \quad (\text{A-5})$$

$$\int_0^x \frac{(1+\varepsilon x)^2}{(1-x)^2} dx = 2\varepsilon(1+\varepsilon) \ln(1-x) + \varepsilon^2 x + \frac{(1+\varepsilon)^2 x}{1-x} \quad (\text{A-6})$$

$$\int_0^x \frac{dx}{(1-x)(\Theta_B - x)} = \frac{1}{\Theta_B - 1} \ln \frac{\Theta_B - x}{\Theta_B (1-x)} \quad \Theta_B \neq 1 \quad (\text{A-7})$$

$$\int_0^x \frac{dx}{ax^2 + bx + c} = \frac{-2}{2ax + b} + \frac{2}{b} \quad \text{for } b^2 = 4ac \quad (\text{A-8})$$

$$\int_0^x \frac{dx}{ax^2 + bx + c} = \frac{1}{a(p-q)} \ln \left( \frac{q}{p} \cdot \frac{x-p}{x-q} \right) \quad \text{for } b^2 > 4ac \quad (\text{A-9})$$

$$\int_0^W (1-aW)^{1/2} dW = \frac{2}{3a} \left[ 1 - (1-aW)^{3/2} \right] \quad (\text{A-10})$$

$$\int_0^\infty (e^{-kt}) \delta(t-\tau) dt = e^{-k\tau} \quad (\text{A-11})$$

## Simpson's five-point formula

$$\int_{x_0}^{x_4} f(x) dx = \frac{h}{3} (f_0 + 4f_1 + 2f_2 + 4f_3 + f_4) \quad h = \frac{X_4 - X_0}{4}$$