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]

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= 4.11x10^{-5} s^{-1} at 20°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°C

Kadar penghidratan etilena oksida (A) kepada etilena glikol $(C_2H_4O + H_2O \rightarrow C_2H_6O_2)$ dalam larutan akuas cair adalah berkadar langsung dengan kepekatan A dan pemalar kadaran k_A = 4.11 × 10^{-5} s^{-1} pada 20°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°C

[6 marks/markah]

[b] An aqueous solution of ethyl acetate (A), with a concentration of 0.30 mol L^{-1} and flowing at 0.50 L s^{-1}, mixes with an aqueous solution of sodium hydroxide (B), of concentration 0.45 mol L^{-1} and flowing at 1.0 L s^{-1}. The combined stream enters a CSTR of volume 500 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 akuas etil asetat (A), dengan kepekatan 0.30 mol L^{-1} mengalir pada 0.50 L s^{-1}, dan bercampur dengan suatu larutan akuas sodium hidroksida (B), yang berkepekatan 0.45 mol L^{-1} dan mengalir pada 1.0 L s^{-1}. Aliran tergabung tersebut memasuki sebuah CSTR yang berisipadu 500 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°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°C and 5 atm. The initial concentration of A is 0.0625 mol/L.

Suatu tindakbalas gas homogen $A \rightarrow 3B$ telah dilaporkan mempunyai kadar pada 215°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°C dan 5 atm dengan suatu suapan yang mengandungi 50% A dan 50% bahan lengai. Kepekatan awal A ialah 0.0625 mol/L.

[8 marks/markah]

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[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

$$A + 3B \rightarrow products$$

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

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

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

$$A + 3B \rightarrow produk$$

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

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

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

$$\left(C_2H_4(g) + \frac{1}{2}O_2(g) \rightarrow C_2H_4O\ (g)\right)$$

[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]

[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→B+C) is carried out in a plug flow reactor. Determine the reaction order, α, and the specific reaction rate constant (k) by using the following data:

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

time (hr) *masa (jam)*	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:

T (K)	273	298	308	318	328	338
k (10^5 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:

[i] $A + B \rightarrow D\text{:}\ \ r_D = k_1 C_A^3 C_B$
$A + B \rightarrow U\text{:}\ \ r_U = k_2 C_A^2 C_B^{0.5}$

[6 marks/markah]

[ii] $A + B \rightarrow D\text{:}\ \ r_D = k_1 C_A^{0.3} C_B^{2.2}$
$A + B \rightarrow U\text{:}\ \ r_U = k_2 C_A^{1.2} C_B^{0.7}$

[6 marks/markah]

...5/-

4. Component A is converted to B in a reactor.
Komponen A ditukarkan kepada B dalam sebuah reaktor.

$$A \rightarrow B$$

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 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 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 melalui imbangan mol, dan imbangan 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 digunalan untuk tindakbalas tersebut pada penukaran 40%, bincangkan isipadu reaktor PFR yang diperlukan berbanding dengan isipadu CSTR yang diperlukan.

[6 marks/markah]

Additional information:

$\Delta H^o_{Rx} = -6900$ J/mol A ,

$k_A/k_B = 3.03$ at 333 K

Activation energy = 65.7 kJ/mol

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

Specific heat capacities:

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

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

Adiabatic energy balance:

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

Maklumat tambahan:

$\Delta H^o_{Rx} = -6900$ J/mol A ,

$k_A/k_B = 3.03$ pada 333 K

Tenaga pengaktifan = 65.7 kJ/mol

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

Haba muatan tentu:

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

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

Imbangan tenaga adiabatik: $X = \dfrac{\sum \Theta_i C_{P_i} (T - T_{i0})}{-\left[\Delta H^o_{Rx}(T_R) + \Delta C_P (T - T_R)\right]}$

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:-

$$I_2 \xrightarrow{k_0} 2I\cdot$$

$$I\cdot + RH \xrightarrow{k_i} R\cdot + HI$$

$$R\cdot + O_2 \xrightarrow{k_{p1}} RO_2\cdot$$

$$RO_2\cdot + RH \xrightarrow{k_{p2}} ROOH + R\cdot$$

$$2RO_2\cdot \xrightarrow{k_t} \text{inactive } \textit{[tidak aktif]}$$

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 dm^3/min. A pulse test gave the following measurements at the outlet:

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

t(min)	0	0.4	1.0	2	3	4	5
C ×10^3 g/dm^3	0	1	3	7.4	9.4	9.7	9.4

t(min)	6	8	10	15	20	25	30
C ×10^3 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]

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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-eights rule

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

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

3. Simpson's quadrature formula

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

Where $h = \dfrac{x_4 - x_0}{4}$

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

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

Where $h = \dfrac{x_N - x_0}{N}$

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

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

Where $h = \dfrac{x_N - x_0}{N}$

Ideal gas constant

$$R = \frac{8.314 \text{ kPa} \cdot .\text{dm}^3}{\text{mol.K}} \qquad R = \frac{1.987 \text{ Btu}}{\text{Ib mol} \cdot {}^\circ \text{R}}$$

$$R = \frac{0.73 \text{ ft}^3 \cdot .\text{atm}}{\text{Ib mol} \cdot {}^\circ \text{R}} \qquad R = \frac{8.3144 \text{ J}}{\text{mol.K}}$$

$$R = \frac{0.082 \text{ dm}^3 \cdot .\text{atm}}{\text{mol.K}} = \frac{0.082 \text{ m}^3 \cdot .\text{atm}}{\text{kmol.K}} \qquad R = \frac{1.987\text{cal}}{\text{mol} \cdot \text{K}}$$

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Useful Integrals in Reactor Design

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

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

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

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

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

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

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

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

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

$$\int_0^W (1-\alpha W)^{1/2}\, dW = \frac{2}{3\alpha}\left[1-(1-\alpha W)^{3/2}\right] \tag{A – 10}$$

$$\int_0^\infty \left(e^{-kt}\right)\delta(t-\tau)\,dt = e^{-kt} \tag{A – 11}$$

Simpson's five-point formula

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