UNIVERSITI SAINS MALAYSIA

First Semester Examination
2010/2011 Academic Session

November 2010

EKC 336 – Chemical Reaction Engineering
[Kejuruteraan Tindak Balas Kimia]

Duration : 3 hours
[Masa : 3 jam]

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

[Sila pastikan bahawa kertas peperiksaan ini mengandungi LAPAN muka surat yang bercetak dan TIGA muka surat Lampiran sebelum anda memulakan peperiksaan ini.]

Instruction: Answer **ALL** (4) questions.

*[**Arahan:** Jawab **SEMUA** (4) soalan.]*

In the event of any discrepancies, the English version shall be used.

[Sekiranya terdapat sebarang percanggahan pada soalan peperiksaan, versi Bahasa Inggeris hendaklah diguna pakai.]

Answer ALL questions.
Jawab SEMUA soalan.

1. [a] Derive the general mol balance equation for plug flow reactor. State all assumptions made in the derivation.

Terbitkan persamaan imbangan mol umum untuk reaktor palam aliran. Nyatakan kesemua andaian yang dibuat dalam terbitan tersebut.

$-r_A$ ≡ rate of reaction, g mol A per cm^3 of liquid per second
ε ≡ volume fraction of gas
F_A ≡ molar flow rate of A, g mol/s
V ≡ volume of reactor

$-r_A$ ≡ kadar tindak balas, g mol A per cm^3 cecair per saat
ε ≡ pecahan isipadu gas
F_A ≡ kadar aliran molar A, g mol/s
V ≡ isipadu reaktor

[5 marks/markah]

[b] The following liquid-phase hydration reaction occurs in a 10,000 L Continous Stirred Tank Reactor (CSTR):
Tindak balas hidrasi fasa cecair berikut berlaku dalam sebuah Reaktor Tangki Teraduk Berterusan (CSTR)berisipadu 10,000 liter.

$$A \xrightarrow{H_2O} B$$

With a first-order rate constant of 2.5 x 10^{-3} min^{-1}.
Dengan satu pemalar kadar tertib pertama 2.5 x 10^{-3} min^{-1}.

[i] What is the steady-state fractional conversion of A if the feed rate is 0.3 L/s and the feed concentration $C_{A,0}$ = 0.12 mol/L?

Berapakah pecahan penukaran keadaan mantap bagi A jika kadar suapan adalah 0.3 L/s dan kepekatan suapan $C_{A,0}$ = 0.12 mol/L?

[ii] If the feed rate suddenly drops to 70% of its original value and is maintained there, what is the fractional conversion of A after 60 minutes, and what is the new steady state fractional conversion?

Jika kadar suapan tiba-tiba jatuh kepada 70% dari nilai asal dan kekal sedemikian, berapakah pecahan penukaran A selepas 60 minit, dan berapakah nilai baru pecahan penukaran dalam keadaan mantap?

[10 marks/markah]

[c] What mass of catalyst is needed to convert 90% of a 150 dm^3 min^{-1} feed consisting of equimolar quantities of reactant and inert, for the gas-phase reaction $2A \rightarrow B$ carried out in a Packed Bed Reactor (PBR) at 3 atm and 50°C (k = 0.1 dm^6 mol^{-1} kg $catalyst^{-1}$ sec^{-1})?

Berapakah jisim pemangkin diperlukan untuk menukar 90% dari suapan berkadar 150 dm^3 min^{-1} *yang mengandungi kuantiti sama molar bahan tindak balas dan bahan lengai, untuk tindak balas fasa gas* $2A \rightarrow B$ *dikendalikan dalam sebuah Reaktor Lapisan Terpadat (PBR) pada 3 atm dan 50°C (k = 0.1* dm^6 mol^{-1} *kg* $pemangkin^{-1}$ s^{-1}*)?*

[5 marks/markah]

[d] The following reaction is important in the chemistry of air pollution:
Tindak balas berikut adalah penting dalam kimia pencemaran udara:

$$NO(g) + O_3(g) \rightarrow NO_2(g) + O_2(g)$$

The frequency factor A= 8.7 x 10^{12} s^{-1} and the rate constant, k, = 300 s^{-1} at 75 °C for the above reaction.
Faktor kekerapan A = 8.7 x 10^{12} s^{-1} *dan pemalar kadar, k = 300* s^{-1}*pada 75 °C untuk tindak balas di atas.*

[i] Find the activation energy (E_a) in Joules per mole for this reaction.
Carikan tenaga pengaktifan (E_a) *dalam Joule per mol untuk tindak balas ini.*

[ii] Find the rate constant (k) of this reaction at 0 °C, assuming E_a to be constant.
Carikan pemalar kadar (k) *bagi tindak balas ini pada 0 °C, dengan mengandaikan* E_a *adalah malar.*

[5 marks/markah]

2. [a] The reaction A → products is studied in the laboratory, and the following data are collected:
Tindak balas A → produk dikaji dalam makmal dan data berikut diperolehi:

Time (s) *Masa (s)*	C_A (M)
0	10
20	8
40	6
60	5
120	3
180	2
300	1

Where C_A is concentration of the A. Determine the reaction order and rate constant using differential method.
Di mana C_A ialah kepekatan A. Tentukan tertib tindak balas dan pemalar kadar dengan menggunakan kaedah pembezaan.

[10 marks/markah]

[b] Answer the following questions by performing a stoichiometric analysis of the gas-phase stoichiometry $2A \rightarrow 2B + C$ for a flow reactor being fed with A containing 75 mol% inert.

Jawab soalan-soalan berikut dengan menjalankan analisa stoikiometri bagi stoikiometri fasa gas $2A \rightarrow 2B + C$ untuk sebuah reaktor aliran disuapkan dengan A yang mengandungi 75 mol% lengai.

[i] Express an elementary rate law in terms of conversion.
Nyatakan satu hukum kadar yang asas dalam sebutan penukaran.

[ii] Calculate the effluent concentration of species C at 90% conversion in terms of C_{A0}.
Kirakan kepekatan keluaran bagi spesis C pada 90% penukaran dalam sebutan C_{A0}.

[iii] Calculate the effluent molar flow rate at 90% conversion in terms of F_{A0}.
Kirakan kadar aliran molar keluaran pada 90% penukaran dalam sebutan F_{A0}.

[10 marks/markah]

[c] Design the minimum volume in order to achieve 95% conversion for a Plug Flow Reactor (PFR) and Continous Stirred Tank Reactor (CSTR) for the kinetic data shown in Figure Q.2.[c].
Rekakan isipadu minima untuk menghasilkan 95% penukaran bagi sebuah Reaktor Aliran Palam (PFR) dan Reaktor Tangki Teraduk Berterusan (CSTR) untuk data kinetik yang ditunjuk dalam Rajah S.2.[c].

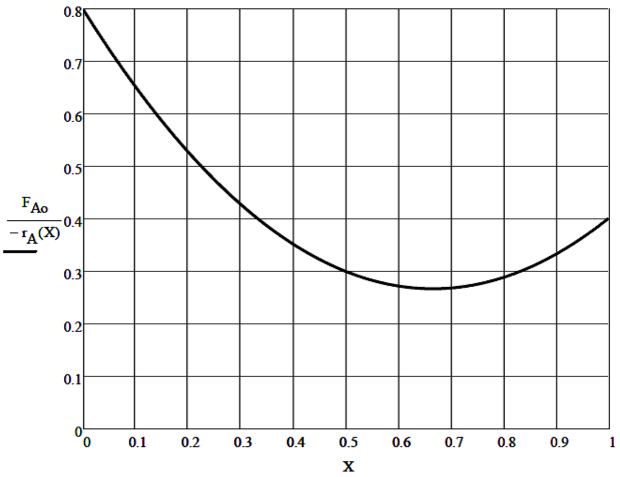

Figure Q.2.[c].
Rajah S.2.[c].

[5 marks/markah]

3. [a] Parallel reactions with following details (where *T* is expressed in K),
Tindak balas selari dengan butiran di bawah ini (di mana T dinyatakan dalam K),

$$A \rightarrow D \qquad -r_{A1} = k_1C_A = 10e^{-4000/T}C_A$$

$$A \rightarrow U_1 \qquad -r_{A2} = k_2 = 20e^{-3000/T}$$

$$A \rightarrow U_2 \qquad -r_{A3} = k_3C_A^2 = 4000e^{-5000/T}C_A^2$$

are required to be carried out in a system where Continuos Stirred Tank Reactor (CSTR) and Plug Flow Rate (PFR) are operated in series at the same temperature in order to achieve maximum selectivity of the desired product D. U_1 and U_2 are undesirable products.

perlu dilakukan dalam Reaktor Tangki Teraduk Berterusan (CSTR) dan Reaktor Aliran Palam (PFR) yang dijalankan secara bersiri pada suhu yang sama untuk mencapai kememilihan maksima untuk produk yang dikehendaki D. U_1 dan U_2 adalah produk yang tidak diingini.

[i] Determine the optimum C_A in terms of k_2 and k_3 to achieve the maximum selectivity of D.

Tentukan C_A optima dalam terma-terma k_2 dan k_3 untuk mencapai kememilihan maksima untuk D.

[6 marks/markah]

[ii] Determine the maximum selectivity and explain whether the maximum selectivity changes with temperature or not.
Tentukan kememilihan maksima dan jelaskan maksima kememilihan berubah dengan suhu atau tidak.

[6 marks/markah]

[b] The second order reaction
Tindak balas urutan kedua

$$2A \rightarrow B + C$$

occurs in the liquid phase. The Residence Time Distribution (RTD) function for the reactor in which it is to be carried out is given in Figure Q.3.[b].

berlaku dalam fasa cecair. Fungsi Agihan Masa Mastautin (RTD) untuk reaktor yang mana tindak balas ini perlu dilakukan adalah seperti dalam Rajah S.3.[b].

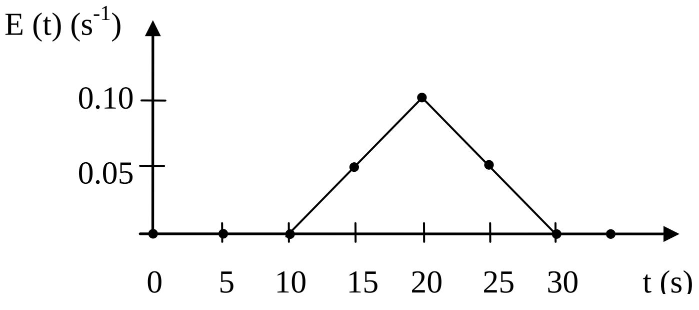

Figure Q.3.[b].
Rajah S.3.[b].

…7/-

The entering concentration is 2 molar and the specific reaction rate is 0.06 dm^3/mol.
Kepekatan suapan adalah 2 molar dan kadar tindak balas tentu reaksi khusus adalah 0.06 dm^3/mol.

[i] Calculate the conversion after 30 s in a batch reactor.
Hitungkan penukaran selepas 30 s di dalam reaktor kelompok.
[6 marks/markah]

[ii] Calculate the conversion that would be achieved in a Continous Stirred Tank Reactor (CSTR) with the same mean residence time, 30 s.

Hitungkan penukaran yang akan dicapai dalam Reaktor Tangki Teraduk Berterusan (CSTR) dengan masa mastautin min yang sama 30 s.
[7 marks/markah]

4. [a] An elementary and irreversible liquid-phase reaction ($D + E \rightarrow F$) is carried out adiabatically in a flow reactor. An equal molar feed in D and E enters at 27°C, and the volumetric flow rate is 2 dm^3/s and $C_{D0} = 0.1$ mol/dm^3. Table Q.4.[a] shows the additional information for this reaction.

Tindak balas fasa cecair dan tidak berbalik ($D + E \rightarrow F$) *dilakukan dalam reaktor adiabatik aliran. Molar suapan yang sama dalam D dan E disuapkan pada 27°C, dan kadar aliran isipadu adalah 2* dm^3/s *dan* $C_{D0} = 0.1$ mol/dm^3. *Jadual S.4.[a] menunjukkan maklumat tambahan untuk tindak balas ini.*

Table Q.4.[a].
Jadual S.4.[a].

Parameters *Parameter-parameter*	Component *Komponen*		
	D	E	F
$H_i^o(273K)$ (kJ/mol)	-20	-15	-41
C_{pi} (J/mol.K)	15	15	30
k (300K) (dm^3/mol.s)	0.01		
E (kJ/mol)	10		

[i] Calculate the Continous Stirred Tank Reactor (CSTR) volume necessary to achieve 85% conversion.
Hitungkan isipadu Reaktor Tangki Teraduk Berterusan (CSTR) yang diperlukan untuk mencapai penukaran 85%.
[12 marks/markah]

[b] The following graph shows the E curve calculated for reactor R:
Graf berikut menunjukkan lengkungan E yang dikira untuk reaktor R:

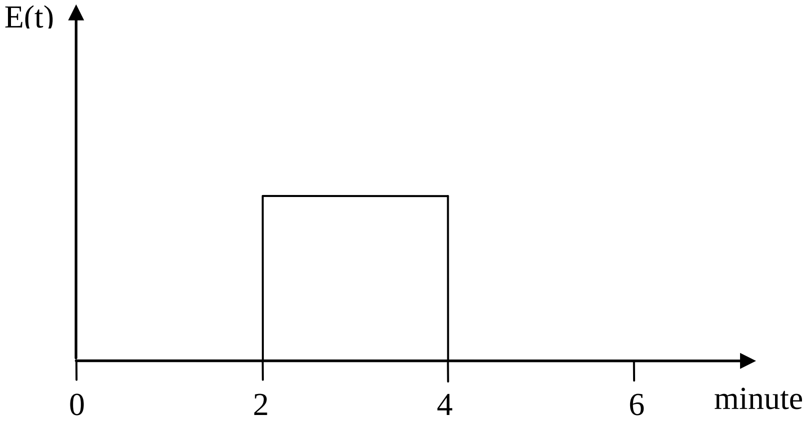

Figure Q.4.[b].
Rajah S.4.[b].

[i] Determine the maximum value of E.
Tentukan nilai maksima E.

[2 marks/markah]

[ii] Determine the fraction of the molecules that spend between 2 and 2.5 minutes in reactor R.
Tentukan pecahan molekul yang berada di antara 2 dan 2.5 minit dalam reaktor R.

[4 marks/markah]

[iii] Draft the curve which corresponds to F(t).
Lakarkan lengkung yang sesuai dengan F(t).

[7 marks/markah]

- ooo O ooo –

Appendix

Useful differential equations:

$$\frac{d}{dx}(uv) = u\frac{dv}{dx} + v\frac{du}{dx}$$

$$\frac{d}{dx}(u/v) = \frac{(v\frac{du}{dx} - u\frac{dv}{dx})}{v^2}$$

Numerical Evaluation of Integrals:

1. Trapezoidal rule

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

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

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

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

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

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

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

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

Ideal gas constant

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

$$R = \frac{1.987\ \text{Btu}}{\text{Ib mol}\cdot{}^{o}\ \text{R}}$$

$$R = \frac{0.73\ \text{ft}^3\cdot.\text{atm}}{\text{Ib mol}\cdot{}^{o}\ \text{R}}$$

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

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

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

First Point

$$\left.\frac{dC_A}{dt}\right|_{t_0} = \frac{-3C_{A0}+4C_{A1}-C_{A2}}{2\Delta t}$$

Interior Points

$$\left.\frac{dC_A}{dt}\right|_{t_i} = \frac{C_{A\,(i+1)}-C_{A(i-1)}}{2\Delta t}$$

Last point

$$\left.\frac{dC_A}{dt}\right|_{t_n} = \frac{C_{A(n-2)}-4C_{A\,(n-1)}+3C_{A(n)}}{2\Delta t}$$

Energy balance:

$$T = T_0 + \frac{X\left[-\Delta H_{Rx}(T_0)\right]}{\Sigma\phi_i\tilde{C}_{Pi}+X\Delta\tilde{C}_P}$$

Rate law:

$$k(T) = k(T_1)e^{\left[\frac{E}{R}\left(\frac{1}{T_1}-\frac{1}{T}\right)\right]}$$

Useful Integrals in Reactor Design

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

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

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

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

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

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

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

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

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

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

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

Simpson's five-point formula

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