

UNIVERSITI SAINS MALAYSIA

Peperiksaan Semester Pertama
Sidang Akademik 1997/98

September 1997

EKC 220/260: Kejuruteraan Tindakbalas Kimia I

Masa: [3 jam]

ARAHAN KEPADA CALON:

Sila pastikan soalan peperiksaan ini mengandungi **SEPULUH (10)** mukasurat bercetak dan **SATU (1)** Lampiran sebelum anda memulakan peperiksaan.

Kertas soalan ini mengandungi **ENAM (6)** soalan.

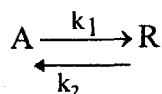
Jawab mana-mana **LIMA (5)** soalan.

Soalan **SATU (1)** mesti dijawab di dalam Bahasa Malaysia.

...2/-

1. [a] Tindakbalas berbalik asas akueus:

The aqueous elementary reversible reaction



berlaku seperti berikut, *proceeds as follows*,

Jadual Table Q1.1

Masa, min <i>Time, min</i>	0	36	65	100	160	∞
C_A , $\frac{\text{mol}}{\text{litre}}$	0.1823	0.1453	0.1216	0.1025	0.0795	0.0494

dengan *with* $C_{A_0} = 0.1823 \frac{\text{mol}}{\text{litre}}$ dan *and* $C_{R_0} = 0$

Dapatkan pemalar kadar k_1 dan k_2 untuk tindakbalas tersebut?

Find the rate constants k_1 and k_2 for the reaction.

(10 markah)

Gunakan formula:

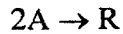
Useful Formula:

$$-\ln \frac{C_A - C_{Ae}}{C_{A_0} - C_{Ae}} = \frac{k_1 t}{\left(1 - \frac{C_{Ae}}{C_{A_0}}\right)}$$

- [b] Bahan tindakbalas tulen bergas, A $\left(C_{A_0} = 100 \frac{\text{millimol}}{\text{litre}}\right)$ disuapkan pada kadar mantap ke dalam CSTR ($V = 0.1$ liter) di mana ia didimerkan (*dimerize*).

Pure gaseous reactant A $\left(C_{A_0} = 100 \frac{\text{millimol}}{\text{litre}}\right)$ is fed at steady rate into a CSTR ($V = 0.1$ litre) where it dimerize

...3/-



Data berikut didapati daripada kadar suapan gas yang berlainan.

For different gas feed rates the following data are obtained.

Jadual (Table) Q1.2

Nombor Ujikaji Run Number	1	2	3	4
v_0 , liter/jam (litre/h)	30.0	9.0	3.6	1.5
$C_{A,out}$ $\frac{\text{millimol}}{\text{litre}}$	85.7	66.7	50	33.3

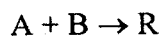
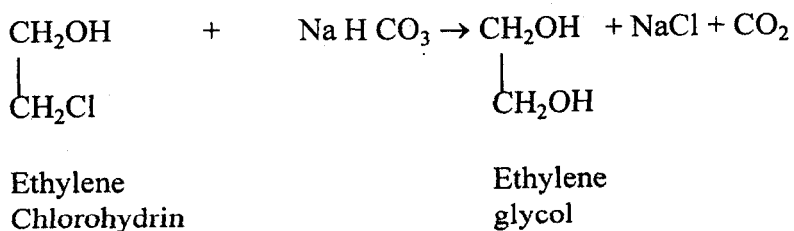
Dapatkan persamaan kadar untuk tindakbalas tersebut. Untuk analisa, tindakbalas ini boleh dianggap sebagai tindakbalas tak berbalik.

Find a rate equation for this reaction. The reaction can be treated as an irreversible reaction for analysis.

(10 markah)

2. Satu tindakbalas asas tidak berbalik dalam fasa cecair ditunjukkan seperti di bawah:

The elementary irreversible liquid phase reaction represented as:



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Tindakbalas ini berlaku pada pemalar kadar $k = 5.2$ liter/mol.jam dan pada suhu $T = 82^\circ\text{C}$. Dua suapan yang tersedia adalah:

takes place at 82°C with rate constant $k = 5.2$ litre/mol. h. The two feeds available are:

[i] 15 wt% larutan akueus "sodium bicarbonate" (Na H CO_3) dan

15 wt% aqueous solution of sodium bicarbonate (Na H CO_3) and

[ii] 30 wt% larutan akueus "ethylene chlorohydrin" $\begin{pmatrix} \text{CH}_2\text{OH} \\ \text{CH}_2\text{Cl} \end{pmatrix}$ yang digunakan untuk pengeluaran "ethylene glycol".

30 wt% aqueous solution of ethylene chlorohydrin $\begin{pmatrix} \text{CH}_2\text{OH} \\ \text{CH}_2\text{Cl} \end{pmatrix}$ to be used for the production of ethylene glycol.

[a] Berapakah isipadu reaktor palam aliran (PFR) yang akan mengeluarkan 20 kg/jam ethylene glycol pada kadar pertukaran 95% daripada suapan sama molar (equimolar) dengan mencampurkan dua aliran suapan pada quantiti yang bersesuaian?

What volume of plug flow reactor (PFR) will produce 20 kg/h ethylene glycol at 95% conversion of an equimolar feed produced by intimately mixing appropriate quantities of the two feed streams.

(12 markah)

[b] Berapakah pula saiz reaktor (CSTR) yang diperlukan untuk suapan, pertukaran dan kadar pengeluaran yang sama seperti di bahagian [a]?

What size of CSTR is needed for the same feed, conversion, and production rate as in part [a]?

(8 markah)

Andaikan semua operasi pada suhu 82°C dan graviti tentu bagi bendalir tindakbalas bercampur ialah 1.02.

...5/-

Assuming all operations at 82°C, and the specific gravity of the mixed reacting fluid is equal to 1.02.

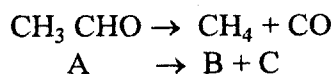
Data:

Data

Komponen	:	Berat molekul
<i>Component</i>	:	<i>Molecular weight</i>
Na H CO ₃		84
CH ₂ OH		
CH ₂ Cl		80.5
CH ₂ OH		
CH ₂ OH		62

3. [a] Satu kajian kinetik telah dibuat untuk penguraian acetaldehyde pada suhu 518°C dan tekanan 1 atm di dalam radas aliran. Ia adalah tindakbalas tak berbalik tertib kedua (*second order*) yang ditunjukkan di bawah:

A kinetic study is made of the decomposition of acetaldehyde at 518°C and 1 atm pressure in a flow apparatus. The reaction is irreversible and second order, represented as:



Wap acetaldehyde (CH₃ CHO) telah dialirkan ke dalam tiub tindakbalas yang dikekalkan pada suhu persekitaran relau, 518°C. Dimensi tiub tindakbalas ialah diameter dalaman = 3.3 cm, panjang = 80 cm dan isipadu, V = 684 cm³. Kadar aliran melalui tiub tersebut diubah-ubahkan dan analisa untuk produk yang dikeluarkan di hujung akhir tiub adalah seperti berikut:

Acetaldehyde (CH₃ CHO) vapors are passed in a reaction tube maintained by a surrounding furnace at 518°C. The reaction tube is 3.3 cm ID and 80 cm long (V = 684 cm³). The flow rate through the tube is varied and analysis of the products from the end of the tube gives the results in Table Q3.

...6/-

Jadual (Table) Q3

Kadar aliran, g/jam <i>Rate of flow, g/h</i>	130	50	21	10.8
Pecahan acetaldehide yang diuraikan <i>Fraction of acetaldehyde decomposed</i>	0.05	0.13	0.24	0.35

Berapakah nilai pemalar kadar?
What is the value of the rate constant?

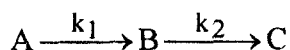
(10 markah)

Data: Berat molekul bagi $\text{CH}_3\text{CHO} = 44$

Useful data: Mol. wt of $\text{CH}_3\text{CHO} = 44$

- [b] Berikut adalah tindakbalas tak berbalik tertib pertama (*first order*) yang berlaku pada ketumpatan molar:

The following irreversible first order reactions occur at constant density:



$$k_1 = 0.15 \text{ min}^{-1}, \quad k_2 = 0.05 \text{ min}^{-1}$$

Berapakah kadar pengeluaran optimum untuk B jika reaktor palam aliran (PFR) berisipadu 10m^3 digunakan? Kadar aliran isipadu suapan ialah $5\text{m}^3/\text{min}$. Komposisi suapan ialah $C_{A_0} = 0.5 \text{ kmol/m}^3$ dan $C_{B_0} = C_{C_0} = 0$.

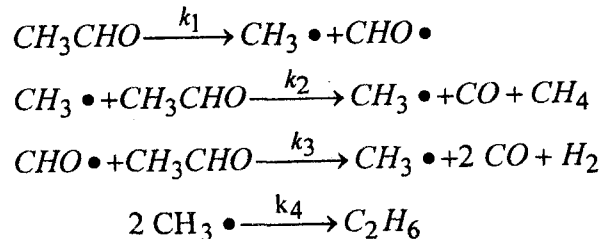
What will be the optimum production rate of B if a plug flow reactor with a volume 10m^3 is used. The volumetric feed flow rate is $5\text{m}^3/\text{min}$ and feed composition is $C_{A_0} = 0.5 \text{ kmol/m}^3$ and $C_{B_0} = C_{C_0} = 0$.

(10 markah)

4. [a] Pirolisis bagi acetaldehyde dipercayai berlaku berdasarkan kepada tindakbalas turutan seperti berikut:

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The pyrolysis of acetaldehyde is believed to take place according to the following sequence of reactions:



Terbitkan hukum kadar untuk kadar penghilangan bagi acetaldehyde, $-r_{\text{AC}}$. Dalam keadaan apakah, ianya boleh dijadikan kepada

Derive the rate law for the rate of disappearance of acetaldehyde, $-r_{\text{AC}}$. Under what conditions does it reduce to

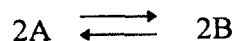
$$-r_{\text{AC}} = k C_{\text{AC}}^{3/2}$$

C_{AC} : Kepekatan acetaldehyde (Concentration of acetaldehyde).

(10 markah)

[b] Satu tindakbalas asas luah haba berbalik (*exothermic*) di dalam fasa gas

The exothermic reversible elementary gas phase reaction



telah dilakukan di dalam reaktor palam aliran (PFR). Tindakbalas tersebut berlaku secara adiabatik. Pada suhu 500K, pemalar keseimbangan ialah 100 dan haba tindakbalas ialah -20.92 kJ/mol bagi A.

is carried out in a PFR. The reaction takes place adiabatically. At 500K, the equilibrium constant is 100, and the heat of reaction is -20.92 kJ/mol of A.

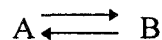
(10 markah)

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Kirakan penukaran keseimbangan sebagai fungsi suhu. Apakah penukaran keseimbangan jika reaktor itu beroperasi pada suhu 1000 K?

Calculate the equilibrium conversion as a function of temperature. What is the equilibrium conversion if the reactor is operated at a temperature of 1000 K.

5. [a] Satu tindakbalas asas berbalik di dalam fasa cecair
The elementary, reversible liquid phase reaction



berlaku di dalam satu reaktor (CSTR) dengan penukar haba (*heat exchanger*). Bahan A tulen dimasukkan ke dalam reaktor.

takes place in a CSTR with a heat exchanger. Pure A enters the reactor.

Terbitkan satu ungkapan untuk mengira $G(T)$, lengkungan haba janaan (*curve*) sebagai fungsi bagi haba tindakbalas, pemalar keseimbangan, suhu dan sebagainya. Oleh itu, tunjukkan juga satu contoh pengiraan untuk $G(T)$ apabila $T = 400\text{K}$.

Derive an expression to calculate $G(T)$, the heat generated curve as a function of heat of reaction, equilibrium constant, temperature etc. Show a sample calculation for $G(T)$ at $T = 400\text{K}$.

Maklumat tambahan:

Additional information:

$$C_{PA} = C_{PB} = 168\text{J/mol.K}$$

$$\Delta H_R = -334.7\text{kJ/mol A}$$

$$K_{eq} = 100\text{ at } 400\text{K}$$

$$k = 1\text{ min}^{-1}\text{ at } 400\text{ K}$$

$$F_{Ao} = 10\text{ mol/min}$$

$$V = 10\text{ dm}^3$$

$$v_o = 1\text{ dm}^3/\text{min}$$

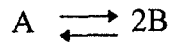
$$\frac{E}{R} = 20,000\text{ K}$$

(8 markah)

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- [b] Satu tindakbalas asas berbalik di dalam fasa gas dilakukan secara adiabatik

The elementary, reversible, gas phase reaction



Kirakan isipadu reaktor dalam aliran (PFR) yang diperlukan untuk mencapai 40% pertukaran. Bahan A tulen disuapkan pada kadar 2 mol/min, pada suhu 100°C dan juga pada kepekatan 0.01 mol/dm³.

is to be carried out adiabatically. Calculate the PFR volume necessary to achieve 40% conversion. Pure A is fed at a rate of 2 mol/min, a temperature of 100°C, and a concentration of 0.01 mol/dm³.

Maklumat tambahan:

Additional information:

$$C_{pA} = 20.0 \text{ J / mol} \cdot ^\circ\text{C}$$

$$C_{pB} = 16.0 \text{ J / mol} \cdot ^\circ\text{C}$$

$$\Delta H_R(100^\circ\text{C}) = -8.37 \text{ kJ / mol}$$

Pemalar keseimbangan, *Equilibrium constant*, $K_c \left(\frac{\text{mol}}{\text{dm}^3} \right)$ ialah is

$$K_c(T) = 0.020 \exp \left[\frac{-8.368}{8.314} \left(\frac{1}{373} - \frac{1}{T} \right) \right]$$

Kadar pemalar, *Rate constant*, $k \text{ (min}^{-1}\text{)}$ ialah is:

$$k(T) = 8241 \exp \left(\frac{-4222}{T} \right)$$

(12 markah)

Gunakan formula:

Useful formula:

$$T = T_o + \frac{(-\Delta H_R^o) X}{\sum \theta_i C_{p_i} + \Delta C_p X}$$

...10/-

6. Analisa agihan masa mastautin (RTD) dijalankan di dalam reaktor fasa cecair. Data berikutan telah direkodkan:

A Residence Time Distribution (RTD) analysis was carried out on liquid phase reactor. The following data are reported:

Jadual Table Q6.

t, saat seconds	c x 10 ³ (g/dm ³)	t, saat seconds	c x 10 ³ (g/dm ³)
0	0	275	8.2
150	0	300	5.0
175	1	325	2.5
200	3	350	1.2
225	7.4	375	0.5
240	9.4	400	0.2
250	9.7	450	0
260	9.4		

- [a] Plotkan lengkung E(t) untuk maklumat tersebut.
Plot the E(t) curve for these data. (8 markah)
- [b] Berapakah pecahan bahan yang berada kurang daripada 250 s di dalam reaktor?
What fraction of the material spends less than 250 s in the reactor? (2 markah)
- [c] Apakah purata masa mastautin (*mean residence time*)?
What is the mean residence time? (5 markah)
- [d] Hidrolisis untuk t-butyl chloride telah dilakukan di dalam reaktor tersebut. Kadar tindakbalas tentu ialah 0.0115 s⁻¹. Apakah penukaran yang diramalkan oleh model pengasingan (*segregation model*) ?
The hydrolysis of t-butyl chloride was carried out in this reactor. The specific reaction rate is 0.0115 s⁻¹. What conversion does the segregation model predict? (5 markah)

LAMPIRAN

Integrasi berguna (pengkamilan):

Useful integral:

$$\int_0^x \left[\frac{1 + \epsilon x}{(1-x)^2} \right] dx = \frac{(1-\epsilon)x}{1-x} - \epsilon \ln \frac{1}{1-x}$$

$$\int_0^X \left(\frac{1 + \epsilon x}{1-x} \right) dx = (1 + \epsilon) \ln \frac{1}{1-X} - \epsilon X.$$

$$\int_0^x \frac{(1 + \epsilon x)^2}{(1-x)^2} dx = 2 \epsilon (1 + \epsilon) \ln (1-x) + \epsilon^2 x + \frac{(1 + \epsilon)^2 x}{1-x}$$

Pemalar gas ideal, R:

Ideal gas constant R:

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

$$R = \frac{8.3144 \text{J}}{\text{mol} \cdot \text{K}} = 1.987 \frac{\text{cal}}{\text{mol} \cdot \text{K}}$$

Integrasi Hukum Simpson (pengkamilan):Simpson's Rule of integrationUntuk titik (point) $N + 1$ di mana $\left(\frac{N}{3} \right)$ ialah integer,For $N + 1$ points, where $\left(\frac{N}{3} \right)$ is an integer,

$$\int_{X_0}^{X_N} f(X) dX = \frac{3}{8} h [f_0 + 3f_1 + 3f_2 + 2f_3 + 3f_4 + 3f_5 + 2f_6 + \dots + 3f_{N-1} + f_N]$$

di mana where $h = \frac{X_N - X_0}{N}$ Untuk titik $N + 1$, di mana N ialah genapFor $N + 1$ points, where N is even

$$\int_{X_0}^{X_N} f(X) dX = \frac{h}{3} (f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \dots + 4f_{N-1} + f_N)$$