UNIVERSITI SAINS MALAYSIA

First Semester Examination
Academic Session 2005/2006

Peperiksaan Semester Pertama
Sidang Akademik 2005/2006

November 2005

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

Duration : 3 hours
[Masa : 3 jam]

Please ensure that this examination paper contains ELEVEN printed pages and TWO printed pages of Appendix before you begin the examination.

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

Instruction: Answer **FOUR (4)** questions. Answer any **TWO (2)** questions from Section A. Answer any **TWO (2)** questions from Section B.

*[**Arahan:** Jawab **EMPAT** (4) soalan. Jawab mana-mana **DUA** (2) soalan dari Bahagian A. Jawab mana-mana **DUA** (2) soalan dari Bahagian B.]*

[Pelajar dibenarkan menjawab semua soalan dalam Bahasa Inggeris ATAU Bahasa Malaysia ATAU kombinasi kedua-duanya.]

...2/-

Section A : Answer any TWO questions.
Bahagian A : Jawab mana-mana DUA soalan.

1. [a] A first order homogeneous reaction of A $\rightarrow$3B is carried out in a constant pressure batch reactor. Starting with pure A the volume after 12 min is increased by 70 percent at a pressure of 1.8 atm. If the same reaction is carried out in a constant volume reactor and the initial pressure is 1.8 atm, calculate the time required to bring the pressure to 2.5 atm.

[11 marks]

[b] [i] The space time necessary to achieve 70 percent conversion in a continuous stirred tank reactor (CSTR) is 3 hrs, determine the reactor volume required to process 4 dm^3 min^{-1}.

[4 marks]

[ii] If the same reaction is carried out in PFR, what is the space velocity for this reactor?

[4 marks]

[c] Write the reaction equation for the following. Identify what type of reaction it is.

[i] Sulfur trioxide and water combine to make sulfuric acid.

[ii] Calcium carbonate heated to leave calcium oxide and carbon dioxide.

[iii] Calcium phosphate and sulfuric acid reacted to make calcium sulfate and phosphoric acid.

[6 marks]

1. [a] Suatu tindakbalas homogen tertib pertama A $\rightarrow$3B dijalankan di dalam sebuah reaktor kelompok tekanan malar. Bermula dengan A tulen, isipadu selepas 12 min meningkat sebanyak 70 peratus pada tekanan 1.8 atm. Jika tindakbalas yang sama dijalankan pada isipadu malar dan tekanan awalnya adalah 1.8 atm, kirakan masa yang diperlukan untuk membawa tekanan kepada 2.5 atm.

[11 markah]

[b] [i] Ruang yang diperlukan untuk mencapai penukaran 70 peratus di dalam reaktor tangki teraduk berterusan (CSTR) adalah 3 jam, tentukan isipadu reaktor yang diperlukan untuk memproses 4 dm^3min^{-1}.

[4 markah]

[ii] Jika tindakbalas yang sama dijalankan di dalam reaktor aliran palam (PFR), berapakah halaju ruang bagi reaktor ini?

[4 markah]

...3/-

[c] Tuliskan persamaan tindakbalas yang berikut. Kenalpasti apakah jenis tindakbalasnya.

[i] Sulfur trioksida dan air bergabung untuk menjadi asid sulfurik.

[ii] Kalsium karbonat dipanaskan untuk menghasilkan kalsium oksida dan karbon oksida.

[iii] Kalsium fosfat dan asid sulfurik bertindakbalas untuk menjadi kalsium sulfat dan asid fosforik.

[6 markah]

2. [a] A plug flow reactor (PFR) operating isothermally at 773 K is used to conduct the following reaction:

methylacetoxypropionate → acetic acid + methyl acrylate

$$A \rightarrow B + C$$

if a feed of pure methylacetoxypropionate enters at 5 atm and at a flow rate of 0.193 dm^3/s, what length of pipe with cross sectional area of 0.0388 cm^2 is necessary for the reaction to achieve 90 % conversion?

Data: $k = 7.8 \times 10^9 \exp [-19{,}200/T]\ s^{-1}$

[10 marks]

[b] A new drug, Slatearium, has tremendous market potential to increase brain function. The reaction rate is measured from previous laboratory studies and is found to be elementary. Slaterarium is formed by mixing Newellium and Dahmium together in a batch reactor at low temperature 162 K with the following stoichiometry:

$$D + N \rightleftharpoons S$$

The reaction rate constants at the recommended reaction temperature of 162 K are

$$k_f = 2 \times 10^{-3} \frac{m^3_{liquid}}{mol.s} \text{ and } k_{reverse} = 5 \times 10^{-4} s^{-1}$$

As in most pharmaceutical operations, the reaction is conducted in batches to guarantee a sterile product. The initial concentrations of Newellium and Dahmium are each 0.5 mol/m^3. Determine the maximum conversion of Newellium that can be obtained in this system.

[10 marks]

...4/-

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

[i] Batch

[ii] Continuous stirred tank

[iii] Plug flow

[5 marks]

2. *[a] Sebuah reaktor aliran palam beroperasi secara isoterma 773 K telah digunakan untuk menjalankan tindakbalas yang berikut:*

metilasetoksipropionat → asid asetik + metil akrilat

$$A \rightarrow B + C$$

Jika suatu suapan metilasetoksipropionat tulen masuk pada 5 atm dan pada kadar aliran 0.193 dm^3/s, apakah panjang paip dengan luas keratan rentas 0.0388 sm^2 yang diperlukan bagi tindakbalas untuk mencapai penukaran 90 % ?

Data: $k = 7.8 \times 10^9 \exp[-19{,}200/T]\ s^{-1}$

[10 markah]

[b] Sejenis ubat baru, Slatearium, mempunyai potensi pemasaran yang besar untuk meningkatkan fungsi otak. Kadar tindakbalas diukur daripada kajian makmal terdahulu dan ditemui sebagai asas. Slateranium terbentuk dengan mencampurkan Newellium dan Dahmium bersama-sama di dalam reaktor berkelompok pada suhu yang rendah 162 K dengan stoikiometri yang berikut:

$$D + N \rightleftharpoons S$$

Pemalar kadar tindakbalas pada suhu tindakbalas yang dicadangkan iaitu 162 K adalah

$$k_f = 2 \times 10^{-3} \frac{m^3_{cecair}}{mol.s} \text{ dan } k_{berbalik} = 5 \times 10^{-4}\ s^{-1}$$

Seperti kebanyakan operasi farmaseutikal, tindakbalas dijalankan secara berkelompok untuk memastikan produk yang steril. Tentukan penukaran maksimum bagi Newellium yang boleh diperolehi daripada sistem ini.

[10 markah]

[c] Apakah kelebihan dan kekurangan reaktor-reaktor yang berikut:

[i] Kelompok

[ii] Tangki teraduk berterusan

[iii] Aliran palam

[5 markah]

...5/-

3. [a] The elementary reaction A + 2B → 2C + D. The reactor is initially charged with $\frac{C_B^0}{C_A^0} = 3.0$, and $C_A^0 = 0.01\,\text{mol/L}$, calculate the value of reaction rate constant, k after 10 min of reaction when the conversion of A is 50 percent.

[10 marks]

[b] Determine the reaction order, and the reaction rate constant for the following data which were obtained at 25°C in a constant-volume batch reactor using pure gaseous A:

$$A \rightarrow 2B$$

Time(min)	Total Pressure (mmHg)
0	215
2	240
4	275
6	320
8	390
10	475
12	600
14	760

[10 marks]

[c] How many type of reactors can be used to determine the rate law? What are the differences between them?

[5 marks]

3. *[a] Tindakbalas asas A + 2B → 2C + D. Reaktor ini pada mulanya dicajkan dengan* $\frac{C_B^o}{C_A^o} = 3.0$, *dan* $C_A^o = 0.01$ *mol/L, kirakan nilai pemalar kadar tindakbalas, k selepas 10 min tindakbalas apabila penukaran A adalah 50 peratus.*

[10 markah]

[b] Tentukan tertib tindakbalas dan pemalar kadar tindakbalas bagi data berikut yang diperolehi pada 25°C di dalam reaktor kelompok isipadu-malar menggunakan gas A tulen:

$$A \rightarrow 2B$$

Masa (min)	*Jumlah Tekanan (mmHg)*
0	*215*
2	*240*
4	*275*
6	*320*
8	*390*
10	*475*
12	*600*
14	*760*

[10 markah]

[c] Berapakah jenis reaktor yang boleh digunakan untuk menentukan hukum kadar? Apakah perbezaan antaranya?

[5 markah]

...6/-

Section B : Answer any TWO questions.
Bahagian B : Jawab mana-mana DUA soalan.

4. [a] The following liquid-phase reactions were performed in a plug flow reactor (PFR),

$$A \rightarrow 2R \qquad (-r_{A1}) = k_1 C_A$$

$$A \rightarrow 3S \qquad (-r_{A2}) = k_2 C_A$$

For a residence time of 40 s the conversion of A was found to be 60% and the ratio of moles of R produced to moles of S produced was found to be 4 to 1. The reactor feed was pure A. Calculate the values of k_1 and k_2.

[12 marks]

[b] A possible free-radical mechanism for the thermal decomposition of acetaldehyde,

$$CH_3CHO \rightarrow CH_4 + CO$$

is as follow:

$$CH_3CHO \xrightarrow{k_1} CH_3^{\bullet} + CHO^{\bullet}$$

$$CHO^{\bullet} \xrightarrow{k_2} CO + H^{\bullet}$$

$$H^{\bullet} + CH_3CHO \xrightarrow{k_3} CH_3CO^{\bullet} + H_2$$

$$CH_3^{\bullet} + CH_3CHO \xrightarrow{k_4} CH_4 + CH_3CO^{\bullet}$$

$$CH_3CO^{\bullet} \xrightarrow{k_5} CH_3^{\bullet} + CO$$

$$2\,CH_3^{\bullet} \xrightarrow{k_6} C_2H_6$$

[i] Which species are the chain carriers?

[ii] Classify each step in the mechanism.

[iii] Derive the rate law from the mechanism above and state the order of reaction predicted. Assume H_2 and C_2H_6 are minor species.

[13 marks]

...7/-

4. [a] *Tindakbalas fasa-cecair yang berikut dijalankan di dalam sebuah reaktor aliran palam (PFR),*

$$A \rightarrow 2R \qquad (-r_{A1}) = k_1 C_A$$

$$A \rightarrow 3S \qquad (-r_{A2}) = k_2 C_A$$

Bagi masa mastautin 40 s, penukaran A didapati sebanyak 60% dan nisbah mol R yang terhasil kepada mol S yang terhasil didapati sebanyak 4:1. Suapan reaktor adalah A tulen. Kirakan nilai k_1 dan k_2.

[12 markah]

[b] *Suatu mekanisma radikal-bebas yang mungkin bagi penguraian suhu bagi asetaldehid,*

$$CH_3CHO \rightarrow CH_4 + CO$$

adalah seperti berikut:

$$CH_3CHO \xrightarrow{k_1} CH_3^{\bullet} + CHO^{\bullet}$$

$$CHO^{\bullet} \xrightarrow{k_2} CO + H^{\bullet}$$

$$H^{\bullet} + CH_3CHO \xrightarrow{k_3} CH_3CO^{\bullet} + H_2$$

$$CH_3^{\bullet} + CH_3CHO \xrightarrow{k_4} CH_4 + CH_3CO^{\bullet}$$

$$CH_3CO^{\bullet} \xrightarrow{k_5} CH_3^{\bullet} + CO$$

$$2\,CH_3^{\bullet} \xrightarrow{k_6} C_2H_6$$

[i] *Spesis-spesis yang manakah pembawa rantai?*

[ii] *Kelaskan setiap langkah di dalam mekanisma di atas.*

[iii] *Terbitkan hukum kadar daripada mekanisma di atas dan nyatakan tertib tindakbalas yang dijangkakan. Anggapkan H_2 dan C_2H_6 adalah spesis minor.*

[13 markah]

...8/-

5. [a] The gas-phase reaction

$$A \rightarrow B + C \qquad (-r_A) = kC_A$$

is to be carried out in a Continuous Stirred Tank Reactor (CSTR) of volume 0.02 m^3. Heat is to be removed from the reactor by cooling coils carrying water at 373 K and discharging saturated steam at 373 K. The feed consists of pure A at a temperature of 325 K and a pressure of 1 bar and flow rate 10^{-3} mol s^{-1}. Calculate the operating temperature and conversion of the steady-state operating points.

Data:

$UA = 5x10^{-2}$ (WK^{-1})

$k = 10^{11} \exp\left(-\frac{18{,}000}{T}\right)$ (s^{-1}) : T is in Kelvin

$\Delta H_R = -70$ kJ/mol of A

$\bar{C}_{PA} = 120$ J/mol K

$\bar{C}_{PB} = 80$ J/mol K

$\bar{C}_{PC} = 40$ J/mol K

R = 8.314 J/mol K

[15 marks]

[b] A first-order, liquid-phase reaction,

$A \rightarrow B$ $\qquad (-r_A) = kC_A$ $\quad k=0.307\ s^{-1}$

is performed in a non-ideal reactor with the reactor residence time distribution (RTD) shown in Table Q. 4. [b] .

Table Q. 4. [b]

t (s)	E (t)
0	0.00
2	0.04
4	0.15
6	0.15
8	0.1
10	0.05
12	0.01
14	0.00

[i] What is the conversion of A?

[ii] Compare the conversion to that of a CSTR and a PFR of the same mean residence time (6 s).

[iii] Comment on the results.

[10 marks]

...9/-

5. [a] *Tindakbalas fasa-gas*

$$A \rightarrow B + C \qquad (-r_A) = kC_A$$

dijalankan di dalam reaktor tangki teraduk berterusan (CSTR) berisipadu 0.02 m^3. Haba disingkirkan daripada reaktor menggunakan lingkaran penyejukan yang membawa air pada 373 K dan mengeluarkan stim tepu pada 373 K. Suapan mengandungi A tulen pada suhu 325 K dan tekanan 1 bar dan kadar aliran 10^{-3} mol s^{-1}. Kirakan suhu operasi dan penukaran bagi titik operasi berkeadaan mantap.

Data:

$UA = 5x10^{-2} \quad (WK^{-1})$

$k = 10^{11} \exp\left(-\frac{18{,}000}{T}\right) \quad (s^{-1}) \quad : T$ *dalam unit Kelvin*

$\Delta H_R = -70$ *kJ/mol bagi A*

$\bar{C}_{PA} = 120$ *J/mol K*

$\bar{C}_{PB} = 80$ *J/mol K*

$\bar{C}_{PC} = 40$ *J/mol K*

$R = 8.314$ *J/mol K*

[15 markah]

[b] *Suatu tindakbalas fasa-cecair, tertib pertama,*

$A \rightarrow B \qquad (-r_A) = kC_A \quad k=0.307\ s^{-1}$

dijalankan di dalam reaktor tak-unggul dengan taburan masa mastautin (RTD) ditunjukkan dalam Jadual S. 4. [b] .

Jadual S. 4. [b]

t (s)	*E (t)*
0	*0.00*
2	*0.04*
4	*0.15*
6	*0.15*
8	*0.1*
10	*0.05*
12	*0.01*
14	*0.00*

[i] *Berapakah penukaran A?*

[ii] *Bandingkan penukaran antara sebuah Reaktor Tangki Teraduk Berterusan (CSTR) dan sebuah reaktor aliran palam (PFR) yang mempunyai masa mastautin purata (6 s).*

[iii] *Beri ulasan terhadap keputusan yang diperolehi.*

[10 markah]

...10/-

6. [a] The gas-phase reaction

$A \rightarrow B \qquad (-r_A) = kP_A$

is to be carried out in an adiabatic PFR. The feed consists of a 50% A and 50% inert at a total flow rate of 6.3 mol/s and a temperature of 300 K. Calculate the reactor volume required for 80% conversion.

Data:

$P = 1$ bar

$k = 28.1 \exp\left(\frac{-E}{RT}\right)$ mol s^{-1} m^{-3} bar

$\Delta H_R = -50$ kJ/mol

$E/R = 1000$ K

$\bar{C}_P = 100$ J/mol K

[15 marks]

[b] A liquid reacts according to $A \rightarrow R$ as it flows through a vessel. If $C_{Ao} = 1$ mol/L and $-r_A = 2C_A^{0.5}$, find the conversion of A for the flow patterns of Figure Q. 6.[b]

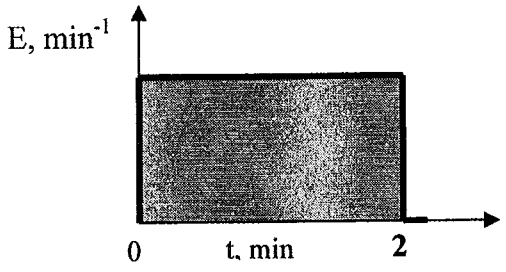


Figure Q. 6. [b]

[10 marks]

6. *[a] Tindakbalas fasa-gas*

$A \rightarrow B \qquad (-r_A) = kP_A$

dijalankan di dalam sebuah reaktor aliran palam (PFR) adiabatik. Suapan mengandungi 50% A dan 50% bahan lengai pada jumlah kadar aliran 6.3 mol/s dan pada suhu 300 K. Kirakan isipadu reaktor yang diperlukan bagi penukaran 80%.

Data:

$P = 1$ *bar*

$k = 28.1 \exp\left(\frac{-E}{RT}\right)$ *mol* s^{-1} m^{-3} *bar*

$\Delta H_R = -50$ *kJ/mol*

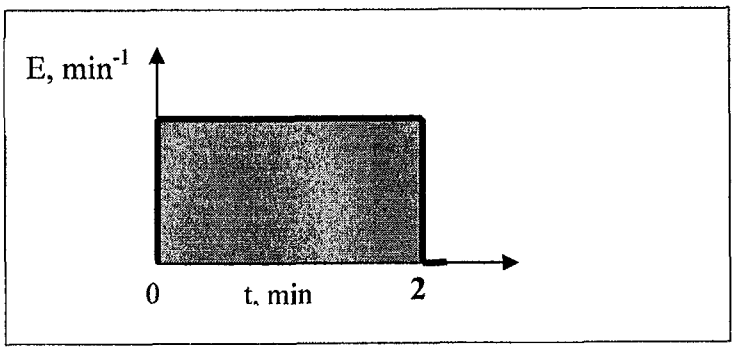
$E/R = 1000$ *K*

$\bar{C}_P = 100$ *J/mol K*

[15 markah]

...11/-

[b] *Suatu cecair bertindakbalas mengikut* $A \rightarrow R$ *apabila ia mengalir melalui sebuah tangki. Jika* $C_{Ao} = 1$ *mol/L dan* $-r_A = 2C_A^{0.5}$, *carikan penukaran A bagi corak aliran dalam Rajah S. 6.[b]*



Rajah S. 6. [b]

[10 markah]

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Lampiran

Useful Integrals in Reactor Design

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

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

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

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

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

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

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

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

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

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

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

Simpson's five-point formula

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

...2/-