UNIVERSITI SAINS MALAYSIA

First Semester Examintaion
Academic Session 2004/2005

Peperiksaan Semester Pertama
Sidang Akademik 2004/2005

October 2004
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EKC 336E – Chemical Reaction Engineering
[Kejuruteraan Tindakbalas Kimia]

Duration : 3 hours
[Masa : 3 jam]

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

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

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

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

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

Answer any <u>FOUR</u> questions.
Jawab mana-mana <u>EMPAT</u> soalan.

1. [a] Two stirred tank reactors are available at a chemical plant, one of volume 100 m^3 and the other of volume 30 m^3. It is suggested that these tanks be used as a two stage CSTR for carrying out an irreversible liquid phase reaction, A + B →Products. The two reactants only will be present in the feed stream in equimolar amounts, $C_{Ao} = C_{Bo} = 1.5$ gmol/dm^3. The volumetric feed rate will be 20 dm^3/min. The reaction is first order with respect to each of the reactants A and B i.e., second order overall. The rate constant is 0.011 dm^3/ (gmol.min). Which tank should be used as the first stage for higher overall conversion?

[15 marks]

[b] Briefly explain why PFR requires smaller volume than CSTR to achieve same conversion for isothermal reaction?

[5 marks]

[c] What assumptions should be made in the derivation of the design equation for:

[i] batch reactor

[ii] CSTR reactor

[iii] Plug Flow Reactor (PFR)

[5 marks]

1. [a] Dua buah reaktor tangki teraduk di dalam sebuah loji kimia, sebuah mempunyai isipadu 100 m^3 dan sebuah lagi mempunyai isipadu 30 m^3. Cadangan telah dibuat supaya tangki-tangki ini digunakan sebagai CSTR dua peringkat untuk menjalankan tindakbalas fasa cecair tak berbalik, A + B → produk. Kedua-dua bahan tindakbalas di dalam aliran suapan adalah dalam jumlah sama molar, $C_{Ao} = C_{Bo} = 1.5$ gmol/dm^3. Jumlah kadar aliran isipadu adalah 20 dm^3/minit. Tindakbalas adalah tertib pertama kepada setiap bahan tindakbalas A dan B iaitu keseluruhan adalah tertib kedua. Pemalar kadar adalah 0.011 dm^3/ (gmol.minit). Tangki yang manakah yang perlu digunakan pada peringkat pertama untuk mencapai penukaran keseluruhan yang lebih tinggi?

[15 markah]

[b] Terangkan secara ringkas mengapa PFR memerlukan isipadu yang lebih kecil berbanding CSTR untuk mencapai penukaran yang sama bagi tindakbalas sesuhu?

[5 markah]

[c] Apakah anggapan yang dibuat bagi menerbitkan persamaan reka bentuk bagi

[i] reaktor kelompok

[ii] reaktor CSTR

[iii] reaktor aliran palam (PFR)

[5 markah]

2. [a] The following aqueous-phase reaction is carried out in a 0.02 m^3 continuous-stirred tank reactor (CSTR):

$$A \text{ (aq)} \rightarrow B \text{ (aq)}$$

The CSTR is fed with dilute aqueous solution containing 0.1 mol/lit of *A* at a total volumetric flow rate of 20 lit/min. The temperature of the feed stream, the outlet stream and fluid inside the CSTR have all been measured and found to be 30°C. The concentration of A in the product stream from the CSTR is measured using on-line UV-spectroscopy to be 0.03 mol/lit. The rate of consumption of species A is known to follow the following first-order rate law:

$$(-r_A) = k\, C_A$$

[i] Calculate the reaction rate $(-r_A)$ for conditions in the CSTR

[5 marks]

[ii] If the same reaction is carried out in a PFR with same feed flow rate and at same temperature, calculate the volume of a PFR required for attaining the same conversion of *A* as that in CSTR described above.

[10 marks]

[b] The following irreversible reaction takes place in a 100 dm^3 CSTR:

$$A \rightarrow B$$

The total initial follow rate is 20 mol/min with initial concentration of A, C_{A0}= 5 mol/dm^3. The feed is 50% A and 50 mol% of inerts. The reactions follow the first order rate law. The rate constant is 0.1 min^{-1}. What is the conversion?

[10 marks]

2. [a] Tindakbalas fasa-akues berikut dijalankan di dalam reaktor tangki teraduk berterusan (CSTR) bersaiz 0.02 m^3

$$A \text{ (ak)} \rightarrow B \text{ (ak)}$$

CSTR disuapkan dengan larutan akues cair mengandungi 0.1 mol/L bagi A pada kadar aliran isipadu 20 L/minit. Suhu aliran suapan, aliran keluar dan bendalir di dalam CSTR semuanya telah diukur dan didapati pada 30°C. Kepekatan A di dalam aliran produk daripada CSTR yang diukur menggunakan spektroskop-UV dalam talian adalah di dapati 0.03 mol/L. Kadar penggunaan spesis A dikenalpasti mengikut hukum kadar tertib pertama yang berikut

$$(-r_A) = k\, C_A$$

...4/-

[i] *Kira kadar tindakbalas ($-r_A$) untuk keadaan di dalam CSTR.*

[5 markah]

[ii] *Jika tindakbalas dijalankan di dalam PFR dengan kadar aliran suapan yang sama dan suhu yang sama, kirakan isipadu PFR yang diperlukan bagi mencapai penukaran A yang sama seperti di dalam CSTR yang digambarkan di atas.*

[10 markah]

[b] *Tindakbalas tak berbalik berikut berlaku di dalam CSTR bersaiz 100 dm^3 :*

$$A \rightarrow B$$

Kadar aliran awal keseluruhan adalah 20 mol/minit dengan kepekatan awal A, C_{A0}= 5 mol/dm^3. Suapan adalah 50% A dan 50 mol% bahan lengai. Tindakbalas mengikut hukum kadar tertib pertama. Pemalar kadar adalah 0.1 per minit. Apakah penukarannya?

[10 markah]

3. [a] The irreversible isomerization

$$A \rightarrow B$$

was carried out in a *batch reactor* and the following concentration-time data were obtained:

t (min)	0	10	20	30	40	50	60
C_A (mol/dm^3)	3.37	2.45	1.74	1.23	0.88	0.62	0.44

By using graphical method, determine the reaction order, α, and the specific reaction rate, *k*?

[15 marks]

[b] For the irreversible gas-phase reaction

$$A \rightarrow 2B$$

being carried out in a constant-pressure batch reactor in which pure A is fed to the reactor. The initial concentration of A is 0.2 g mol/L and the rate of reaction is

$$\frac{10^{-2}}{-r_A} = 3.0\frac{m^3 \cdot s}{mol}$$

what length of time is necessary to achieve 40 % conversion?

[10 marks]

3. [a] *Pengisomeran tak berbalik*

$$A \rightarrow B$$

dijalankan di dalam reaktor berkelompok dan data kepekatan-masa berikut diperolehi:

t (minit)	0	10	20	30	40	50	60
C_A (mol/dm^3)	3.37	2.45	1.74	1.23	0.88	0.62	0.44

Dengan menggunakan kaedah graf, tentukan tertib tindakbalas, α, dan kadar tindakbalas tentu, k.

[15 markah]

[b] *Bagi tindakbalas fasa-gas tak berbalik*

$$A \rightarrow 2B$$

dijalankan di dalam reaktor kelompok tekanan-malar di mana bahan tulen disuapkan ke dalam reaktor. Kepekatan awal A adalah 0.2 g mol/L dan kadar tindakbalas adalah:

$$\frac{10^{-2}}{-r_A} = 3.0\frac{m^3 \cdot s}{mol}$$

Apakah tempoh masa yang diperlukan untuk mencapai penukaran 40%?

[10 markah]

4. [a] A first-order, liquid-phase, endothermic reaction, $A \rightarrow B + C$, takes place in a CSTR operating at steady-state. If the feed temperature (T_o) is 310 K, at what temperature (T_C) must a heating coil in the tank be maintained in order to achieve a conversion (X_A) of 0.75?

Given (Arrhenius parameters) $A = 3.5 \times 10^{13}\ s^{-1}$, $E_A = 100{,}000$ J/mol

$\mu = 8.3$ L/s; $V = 15{,}000$ L; $C_{Ao} = 0.80$ mol/L; $\Delta H_{RA} = 51{,}000$ J/mol;

$\rho = 950$ g/L; $C_P = 3.5$ J/g K; $UA = 10{,}000$ J/s K

[15 marks]

[b] Suppose species A undergoes (liquid-phase) reaction according to the following kinetics scheme:

Reaction	Desired	Rate Law	Activation Energy
$A \rightarrow B$	No	$r_B = k_1 C_A$	E_A
$2A \rightarrow C$	Yes	$r_C = k_2 C_A^2$	$E_C < E_A$

Explain briefly each of the following cases:

[i] Does a favorable product distribution result from relatively high or relatively low C_A?

[ii] Does a favorable product distribution result from relatively high or low temperature?

[iii] Does a favorable (i.e. small) reactor size result from high or low C_A? Does a favorable reactor size result from high or low temperature?

[iv] What type of reactor, PFR or single-stage CSTR, should be chosen for this situation, and should it operated at high, low, or optimum T to achieve favorable product distribution consistent with small size of reactor?

[10 marks]

4. [a] *Tertib pertama, fasa cecair, tindakbalas endotermik $A \rightarrow B + C$, berlaku di dalam CSTR yang beroperasi pada keadaan mantap. Jika suhu suapan (T_o) adalah 310 K, pada suhu berapakah (T_C) gegelung pemanas mesti disenggarakan untuk mencapai penukaran (X_A) sebanyak 0.75?*

Diberi (parameter Arrhenius) $A = 3.5x10^{13}\ s^{-1}$, $E_A = 100{,}000$ J/mol

$\mu = 8.3$ L/s; $V = 15{,}000$ L; $C_{Ao} = 0.80$ mol/L; $\Delta H_{RA} = 51{,}000$ J/mol;

$\rho = 950$ g/L; $C_P = 3.5$ J/g K; $U A = 10{,}000$ J/s K

[15 markah]

[b] *Sekiranya spesis A mengalami tindakbalas (fasa cecair) menurut skema kinetik yang berikut:*

Tindakbalas	*Diingini*	*Hukum Kadar*	*Tenaga Pengaktifan*
$A \rightarrow B$	*Tidak*	$r_B = k_1 C_A$	E_A
$2A \rightarrow C$	*Ya*	$r_C = k_2 C_A^2$	$E_C < E_A$

Terangkan secara ringkas kes-kes yang berikut:

[i] Adakah taburan produk yang dikehendaki terhasil dengan menggunakan C_A yang secara relatifnya tinggi atau rendah?

[ii] Adakah taburan produk yang dikehendaki terhasil dengan menggunakan suhu yang secara relatifnya tinggi atau rendah?

[iii] Adakah saiz reaktor yang dikehendaki (iaitu kecil) terhasil dengan menggunakan C_A yang tinggi atau rendah? Adakah saiz reaktor yang dikehendaki terhasil dari suhu yang tinggi atau rendah?

[iv] Apakah jenis reaktor, PFR atau CSTR satu peringkat, yang patut dipilih bagi situasi ini dan patutkah ianya beroperasi pada T tinggi, rendah atau optimum untuk mencapai pembahagian produk yang dikehendaki secara konsisten dengan saiz reaktor yang kecil.

[10 markah]

5. A highly exothermic irreversible reaction, $A + 2B \rightarrow 2C + D$ is conducted in adiabatic CSTR. What is the reactor volume and space time necessary to achieve 35% conversion of A? The reaction rate is first order in A and second order in B.

Data:

ΔH_R = -370.1 kJ/mol	T_o = 303 K
C_{PA}= 84.5 J/(mol-K)	F_{Ao} = 10 mol/min
C_{PB} = 137 J/(mol-K)	F_{Bo} = 30 mol/min
C_{PC} = 170 J/(mol-K)	v = 1000 L/min
C_{PD} = 75 J/(mol-K)	$C_{Bo} = C_{Ao}$ = 0.01 mol/L

$$k = 0.090\exp\left[\frac{(40\text{kJ/mol})}{R}\left(\frac{1}{303} - \frac{1}{T}\right)\right] \quad (\text{L/mol})^2(\text{min})^{-1}$$

[25 marks]

5. *Satu tindakbalas tak berbalikyang sangat eksotemik, $A + 2B \rightarrow 2C + D$ dijalankan di dalam CSTR adiabatik. Apakah isipadu reaktor dan masa ruang yang diperlukan untuk mencapai 35% penukaran A? Kadar tindakbalas adalah tertib pertama bagi A dan tertib kedua bagi B.*

Data:

ΔH_R = -370.1 kJ/mol	T_o = 303 K
C_{PA}= 84.5 J/(mol-K)	F_{Ao} = 10 mol/minit
C_{PB} = 137 J/(mol-K)	F_{Bo} = 30 mol/minit
C_{PC} = 170 J/(mol-K) ·	v = 1000 L/minit
C_{PD} = 75 J/(mol-K)	$C_{Bo} = C_{Ao}$ = 0.01 mol/L

$$k = 0.090\exp\left[\frac{(40\text{kJ/mol})}{R}\left(\frac{1}{303} - \frac{1}{T}\right)\right] \quad (L/mol)^2(minit)^{-1}$$

[25 markah]

6. [a] Consider the nonideal reactor characterized by the RTD data given in Table Q.6:

Table Q. 6

T (min)	C(g/m^3)	E(t) (min^{-1})
0	0	0
1	1	0.02
2	5	0.1
3	8	0.16
4	10	0.2
5	8	0.16
6	6	0.12
7	4	0.08
8	3	0.06
9	2.2	0.044
10	1.5	0.03
12	0.6	0.012
14	0	0

The irreversible gas-phase nonelementary reaction:

$$A + B \rightarrow C + D$$

is a first-order in A and second order in B and is to carried out isothermally. Calculate the conversion for a laminar flow reactor with complete segregation. Additional information:

$C_{Ao} = C_{Bo} = 0.0313$ mol/dm^3	V = 1000 dm^3
$V_o = 10$ dm^3/s	k = 175 dm^6/mol^2 at 320 K

[20 marks]

[b] The decomposition of ozone dramatically changes in the presence of chlorine atoms (catalyst):

$$Cl + O_3 \xrightarrow{k_1} O_2 + ClO$$

$$ClO + O \xrightarrow{k_2} O_2 + Cl$$

$$O + O_3 \rightarrow 2O_2$$

Show that: $$r_C = \frac{k_1 k_2 [Cl]_o [O][O_3]}{k_2[O] + k_1[O_3]}$$

[5 marks]

6. [a] *Pertimbangkan reaktor tak unggul yang dicirikan menggunakan data RTD yang diberi dalam Jadual S.6:*

Jadual S.6

T (minit)	$C (g/m^3)$	$E(t)$ (minit^{-1})
0	0	0
1	1	0.02
2	5	0.1
3	8	0.16
4	10	0.2
5	8	0.16
6	6	0.12
7	4	0.08
8	3	0.06
9	2.2	0.044
10	1.5	0.03
12	0.6	0.012
14	0	0

Tindakbalas tak-asas fasa gas tak berbalik:

$$A + B \rightarrow C + D$$

adalah tertib pertama bagi A dan tertib kedua bagi B dan dijalankan secara sesuhu. Kirakan penukaran bagi reaktor aliran laminar dengan pengasingan sempurna.

Maklumat tambahan :

$C_{Ao} = C_{Bo} = 0.0313\ mol/dm^3$	$V = 1000\ dm^3$
$V_o = 10\ dm^3/s$	$k = 175\ dm^6/mol^2$ pada 320 K

[20 markah]

[b] *Penguraian ozon berubah secara dramatik di dalam kehadiran atom klorin (mangkin):*

$$Cl + O_3 \xrightarrow{k_1} O_2 + ClO$$

$$ClO + O \xrightarrow{k_2} O_2 + Cl$$

$$O + O_3 \rightarrow 2O_2$$

Tunjukkan: $$r_C = \frac{k_1 k_2 [Cl]_o [O][O_3]}{k_2 [O] + k_1 [O_3]}$$

[5 markah]

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Lampiran

Useful Integrals in Reactor Design

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

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

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

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

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

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

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

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

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

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

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

Simpson's five-point formula

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