
UNIVERSITI SAINS MALAYSIA

First Semester Examination
Academic Session 2004/2005

*Peperiksaan Semester Pertama
Sidang Akademik 2004/2005*

October 2004
Oktober 2004

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 FOUR questions.

Jawab mana-mana EMPAT 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, $A + B \rightarrow \text{Products}$. The two reactants only will be present in the feed stream in equimolar amounts, $C_{A0} = C_{B0} = 1.5 \text{ gmol/dm}^3$. The volumetric feed rate will be $20 \text{ dm}^3/\text{min}$. The reaction is first order with respect to each of the reactants A and B i.e., second order overall. The rate constant is $0.011 \text{ dm}^3/(\text{gmol}\cdot\text{min})$. 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, $A + B \rightarrow \text{produk}$. Kedua-dua bahan tindakbalas di dalam aliran suapan adalah dalam jumlah sama molar, $C_{A0} = C_{B0} = 1.5 \text{ gmol/dm}^3$. Jumlah kadar aliran isipadu adalah $20 \text{ dm}^3/\text{minit}$. Tindakbalas adalah tertib pertama kepada setiap bahan tindakbalas A dan B iaitu keseluruhan adalah tertib kedua. Pemalar kadar adalah $0.011 \text{ dm}^3/(\text{gmol}\cdot\text{minit})$. 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?

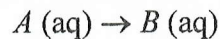
[5 markah]

- [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):



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:



The total initial flow rate is 20 mol/min with initial concentration of A , $C_{A0} = 5 \text{ mol/dm}^3$. 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*



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 :



Kadar aliran awal keseluruhan adalah 20 mol/minit dengan kepekatan awal A, $C_{A0} = 5 \text{ mol/dm}^3$. 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



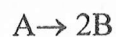
was carried out in a *batch reactor* and the following concentration-time data were obtained:

t (min)	0	10	20	30	40	50	60
$C_A \text{ (mol/dm}^3\text{)}$	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



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

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

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

[10 marks]

...5/-

3. [a] Pengisomeran tak berbalik



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



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_0) 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) $A = 3.5 \times 10^{13} \text{ s}^{-1}$, $E_A = 100,000 \text{ J/mol}$

$$\mu = 8.3 \text{ L/s}; V = 15,000 \text{ L}; C_{A0} = 0.80 \text{ mol/L}; \Delta H_{RA} = 51,000 \text{ J/mol};$$

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

[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:

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- [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_0) adalah 310 K, pada suhu berapakah (T_C) gegelung pemanas mesti disenggarakan untuk mencapai penukaran (X_A) sebanyak 0.75?*

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

$\mu = 8.3 \text{ L/s}$; $V = 15,000 \text{ L}$; $C_{A0} = 0.80 \text{ mol/L}$; $\Delta H_{RA} = 51,000 \text{ J/mol}$;

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

[15 markah]

- [b] *Sekiranya spesies 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:

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

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

[25 marks]

5. *Satu tindakbalas tak berbalik yang 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:

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

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

[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:

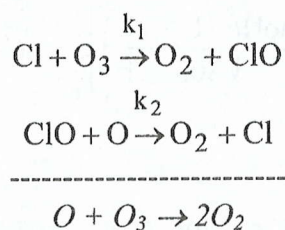


is a first-order in A and second order in B and is to be carried out isothermally. Calculate the conversion for a laminar flow reactor with complete segregation. Additional information:

$C_{A0} = C_{B0} = 0.0313 \text{ mol/dm}^3$	$V = 1000 \text{ dm}^3$
$V_0 = 10 \text{ dm}^3/\text{s}$	$k = 175 \text{ dm}^6/\text{mol}^2 \text{ at } 320 \text{ K}$

[20 marks]

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



Show that:
$$r_C = \frac{k_1 k_2 [\text{Cl}]_0 [\text{O}] [\text{O}_3]}{k_2 [\text{O}] + k_1 [\text{O}_3]}$$

[5 marks]

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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:



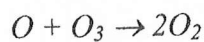
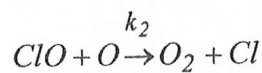
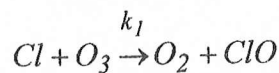
adalah tertib pertama bagi A dan tertib kedua bagi B dan dijalankan secara sesuhu. Kirakan penukaran bagi reaktor aliran laminar dengan pengasingan sempurna.

Maklumat tambahan :

$C_{A0} = C_{B0} = 0.0313 \text{ mol/dm}^3$	$V = 1000 \text{ dm}^3$
$V_o = 10 \text{ dm}^3/\text{s}$	$k = 175 \text{ dm}^6/\text{mol}^2 \text{ pada } 320 \text{ K}$

[20 markah]

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



Tunjukkan:
$$r_C = \frac{k_1 k_2 [\text{Cl}]_o [\text{O}][\text{O}_3]}{k_2 [\text{O}] + k_1 [\text{O}_3]}$$

[5 markah]

Lampiran

Useful Integrals in Reactor Design

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

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

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

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

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

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

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

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

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

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

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

Simpson's five-point formula

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

$$h = \frac{X_4 - X_0}{4}$$