UNIVERSITI SAINS MALAYSIA

First Semester Examination
2014/2015 Academic Session

December 2014 / January 2015

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

Duration : 3 hours
[Masa : 3 jam]

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

[Sila pastikan bahawa kertas peperiksaan ini mengandungi SEMBILAN 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.

1. [a] The gas phase reaction is to be carried out isothermally for the following reaction.

$$\frac{1}{2}N_2 + \frac{3}{2}H_2 \rightarrow NH_3$$

The molar feed is 50% hydrogen and 50% nitrogen, at a pressure of 16.4 atm and 500 K.

[i] Construct a complete stoichiometric table.

[5 marks]

[ii] Compute the value of C_{AO}, δ and ε. Calculate the concentrations of ammonia and hydrogen when the conversion of hydrogen is 80%.

[8 marks]

[iii] Assume the reaction is elementary with $k_{nitrogen}$ = 40 dm^3/mol.s. Determine the rate of reaction solely as a function of conversion for:

[iii].[i]. a flow system.

[4 marks]

[iii].[ii]. a constant volume batch reactor.

[4 marks]

[b] Define the following terms:

[i] Rate law

[2 marks]

[ii] Elementary reaction

[2 marks]

Jawab SEMUA soalan.

1. [a] *Tindak balas fasa gas dijalankan secara sesuhu bagi tindak balas berikut.*

$$\frac{1}{2}N_2 + \frac{3}{2}H_2 \rightarrow NH_3$$

Suapan molar ialah 50% hidrogen dan 50% nitrogen, pada tekanan 16.4 atm dan 500 K.

[i] *Binakan jadual stoikiometri yang lengkap.*

[5 markah]

[ii] *Kirakan nilai C_{AO}, δ dan ε. Kirakan kepekatan ammonia dan hidrogen apabila penukaran hidrogen adalah 80%.*

[8 markah]

[iii] *Anggapkan tindak balas adalah asas dengan $k_{nitrogen} = 40\ dm^3/mol.s$. Tentukan kadar tindak balas sebagai fungsi penukaran sahaja untuk*

[iii].[i]. *suatu sistem aliran*

[4 markah]

[iii].[ii] *suatu reaktor berkelompok berisipadu tetap*

[4 markah]

[b] *Takrifkan terma-terma berikut;*

[i] *Hukum kadar*

[2 markah]

[ii] *Tindak balas asas*

[2 markah]

2. [a]

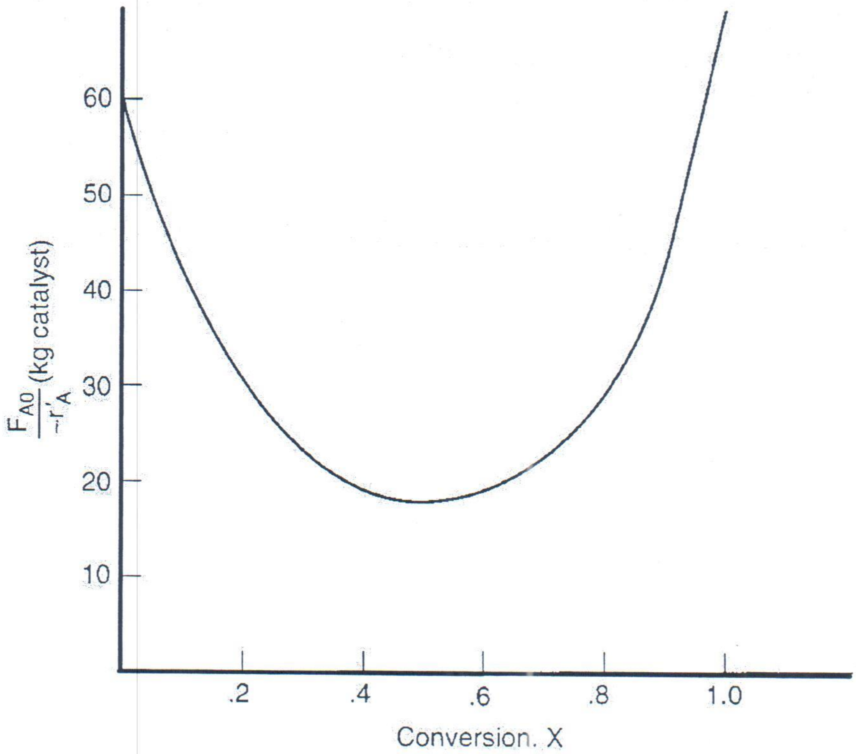


Figure Q.2.[a]: Levenspiel plot for an adiabatic exothermic reaction

The curve shown in the Figure Q.2.[a] is a typical gas-solid catalytic exothermic reaction carried out adiabatically. By using the Figure Q.2.[a]:

[i] Determine the catalyst weight required to achieve 80% conversion in a fluidized CSTR.

[2 marks]

[ii] Determine the catalyst weight required to achieve 80% conversion in a PBR.

[2 marks]

[iii] Provide the best possible reactors arrangement if the reaction is to be carried out in a fluidized CSTR and a PBR containing equal weight of catalyst. The reaction must achieve 60% conversion with the minimum use of the catalyst weight.

[3 marks]

[iv] Determine is the catalyst weight required to achieve 40% conversion in a fluidized CSTR.

[2 marks]

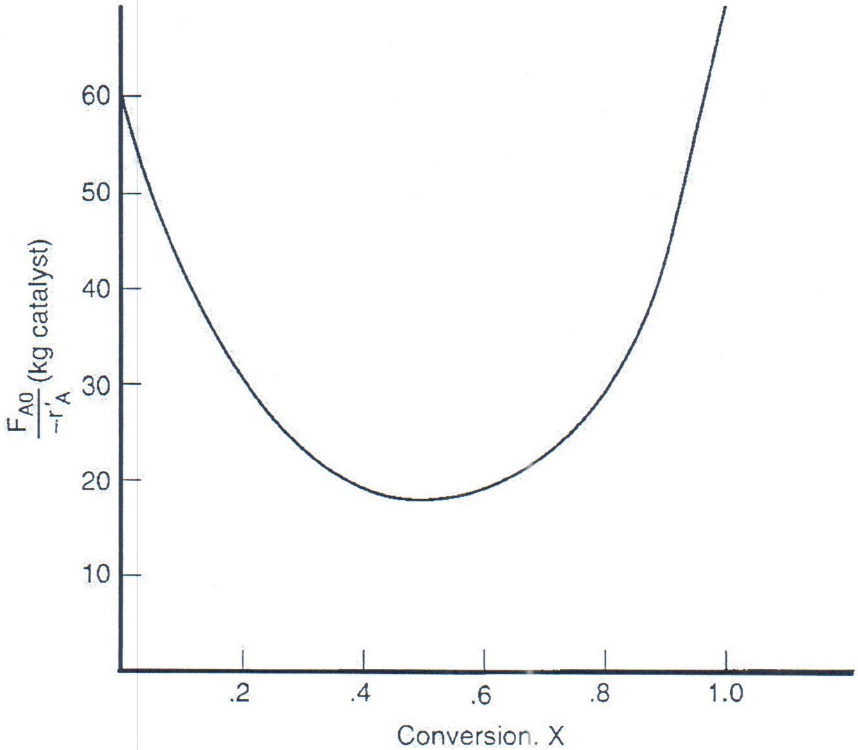
[v] Determine the catalyst weight required to achieve 40% conversion in a PBR.

[2 marks]

[vi] Compare your answers in [iv] and [v] and justify the outcome.

[2 marks]

2. [a]



Rajah S.2.[a]. Plot Levenspiel untuk tindak balas adiabatik luah haba.

Lengkung yang ditunjukkan dalam Rajah S.2.[a]. adalah tindak balas biasa gas-pepejal luah haba yang bermangkin dan dijalankan secara adiabatik. Dengan menggunakan Rajah S.2.[a]:

[i] *Tentukan berat mangkin yang diperlukan untuk mencapai 80% penukaran dalam CSTR terbendalir.*

[2 markah]

[ii] *Tentukan berat mangkin yang diperlukan untuk mencapai 80% penukaran di dalam PBR.*

[2 markah]

[iii] *Berikan susunan reaktor yang paling baik jika tindak balas akan dijalankan dalam CSTR terbendalir dan PBR yang mengandungi berat mangkin yang setara. Tindak balas mesti mencapai 60% penukaran dengan penggunaan mangkin yang minimum.*

[3 markah]

[iv] *Tentukan berat mangkin yang diperlukan untuk mencapai 40% penukaran dalam CSTR terbendalir.*

[2 markah]

[v] *Tentukan berat mangkin yang diperlukan untuk mencapai 40% penukaran dalam PBR.*

[2 markah]

[vi] *Bandingkan jawapan [iv] dan [v], justifikasikan hasilnya.*

[2 markah]

[b] Hydrogen iodide decomposes to form a mixture of a hydrogen and iodine as the following reaction:

$$2HI \rightarrow H_2 + I_2$$

Supposed you have known concentration of HI in a closed reaction vessel kept at 420°C as given in Table Q.2.[b]. Determine the order of reaction and the rate constant.

Table Q.2.[b]. Kinetic data for decomposition of HI

Time (min)	0	5	10	25
Concentration of HI (mol/L)	1.00	0.63	0.46	0.25

[12 marks]

3. [a] An engineer is keen to compare the selectivity of product *B* in two types of reactor, namely CSTR and PFR at 90 % conversion of reactant *A*. The parallel reactions start with an initial concentration of 4 mol A/L.

$$A \rightarrow B,\ r_1 = k_1 = 2$$
$$A \rightarrow C,\ r_2 = k_2 C_A = C_A$$

where rates are in mol.L^{-1}.min^{-1}

[i] From the mass-balance, calculate the residence time for a CSTR until 90 % of A is consumed. Then, determine the selectivity of *B* in the CSTR.

[7 marks]

[ii] From the mass-balance, calculate the residence time for a PFR until 90 % of A is consumed. Determine the selectivity of *B* in the PFR.

[8 marks]

[iii] Determine the type of reactor to be selected. Justify the selection of the reactor type.

[2 marks]

[b] For an adiabatic reactor, a reaction with ΔH_R = - 20 kcal/mol, ρC_p = 1000 cal.L^{-1}.K^{-1} was conducted $A \rightarrow B$. The initial temperature is 300 K while the initial concentration of *A* is 4 mol/L.

[i] Derive the simplest form of energy balance for this adiabatic reactor.
(Useful equation: $T = T_0 + \dfrac{(-\Delta H_R)X}{\sum \Theta_i Cp_i}$)

[4 marks]

[ii] Determine maximum temperature achieved by this reactor.

[2 marks]

[b] *Hidrogen iodida mengurai untuk membentuk campuran hidrogen dan iodin seperti tindak balas berikut:*

$$2HI \rightarrow H_2 + I_2$$

Katakan anda telah mengetahui kepekatan HI dalam kebuk tindak balas bertutup pada 420°C seperti yang diberikan dalam Jadual S.2.[b]. Tentukan tertib tindak balas dan pemalar kadar.

Jadual S.2.[b]. Data kinetik bagi penguraian HI

Masa (min)	0	5	10	25
Kepekatan HI (mol/L)	1.00	0.63	0.46	0.25

[12 markah]

3. [a] *Seorang jurutera berminat untuk membandingkan pemilihan produk* B *yang terbentuk dalam dua jenis reaktor, iaitu CSTR dan PFR pada penukaran 90% daripada bahan tindak balas* A. *Tindak balas selari bermula dengan kepekatan awal dari 4 mol A / L.*

$$A \rightarrow B, r_1 = k_1 = 2$$
$$A \rightarrow C, r_2 = k_2C_A = C_A$$

di mana kadar adalah dalam mol.L^{-1}.min^{-1}

[i] *Daripada imbangan jisim, hitungkan masa mastautin untuk CSTR sehingga 90% daripada* A *digunakan. Kemudian, tentukan pemilihan* B *dalam CSTR.*

[7 markah]

[ii] *Daripada imbangan jisim, hitungkan masa mastautin untuk PFR sehingga 90% daripada* A *digunakan. Tentukan pemilihan* B *dalam PFR.*

[8 markah]

[iii] *Tentukan jenis reaktor yang akan dipilih. Justifikasikan pemilihan jenis reaktor tersebut.*

[2 markah]

[b] *Dalam suatu reaktor adiabatik, tindak balas dengan ΔH_R = - 20 kcal/mol, ρC_p = 1000 cal.L^{-1}.K^{-1} telah dijalankan $A \rightarrow B$. Suhu awal ialah 300 K manakala kepekatan awal adalah 4 mol/L.*

[i] *Terbitkan imbangan tenaga yang paling ringkas untuk reaktor adiabatik ini. (Persamaan yang berguna: $T = T_0 + \frac{(-\Delta H_R)X}{\sum \Theta_i Cp_i}$))*

[4 markah]

[ii] *Tentukan suhu maksimum yang boleh dicapai oleh reaktor ini.*

[2 markah]

[iii] Does the maximum temperature apply to various types of reactor? Yes or No. Justify your answer. *[2 marks]*

4. [a] Table Q.4.[a] represents a continuous response to a pulse input into a tank reactor.

Table Q.4.[a]

Time t, min	0	5	10	15	20	25	30	35
C_{pulse}, g/L fluid	0	3	5	5	4	2	1	0

[i] Tabulate and plot the residence-time distribution (RTD) function, *E(t)*. *[10 marks]*

[ii] Calculate the mean residence time of fluid in the vessel. *[5 marks]*

[iii] RTD can be applied to diagnose problem in the reactors. From your plot in 4.[a].[i], can you analyze the major mixing problems in the tank reactor? *[3 marks]*

[b] In a batch reactor, assume that dispersed noncoalescing droplets react as they pass through a contactor. The initial concentration of A is 2 mol/L. The information of this reaction is given as below:

$$A \rightarrow B\,,\ -r_A = kC_A^2,\ k = 0.5\ \text{L.mol}^{-1}.\text{min}^{-1}$$

[i] Determine the average concentration of A remaining in the droplets leaving the contactor if their RTD is given in Figure Q.4.[b].

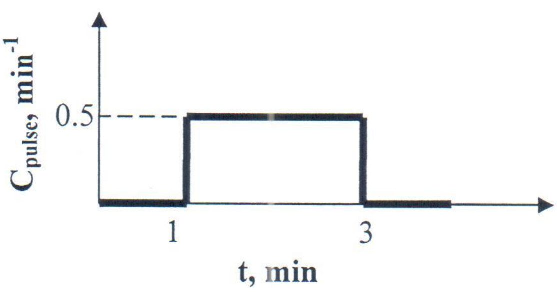


Figure Q.4.[b]

Hint: Apply the segregation model ($\overline{X} = \int_0^\infty X(t)E(t)dt$).

[5 marks]

[ii] If the reaction is first order, does the extent of micromixing affect the mean conversion? Yes or No. Justify your answer. *[2 marks]*

[iii] *Adakah perubahan suhu ini berlaku untuk pelbagai jenis reaktor? Ya atau Tidak. Justifikasikan jawapan anda.*

[2 markah]

4. *[a]* *Jadual S.4.[a] menunjukkan sambutan yang berterusan kepada input denyut ke dalam suatu reaktor tangki.*

Jadual S.4.[a]

Masa t, min	*0*	*5*	*10*	*15*	*20*	*25*	*30*	*35*
C_{denyut}, *g/L cecair*	*0*	*3*	*5*	*5*	*4*	*2*	*1*	*0*

[i] *Jadual dan plotkan taburan masa mastautin (RTD),* E(t).

[10 markah]

[ii] *Kirakan masa mastautin purata cecair di dalam bekas.*

[5 markah]

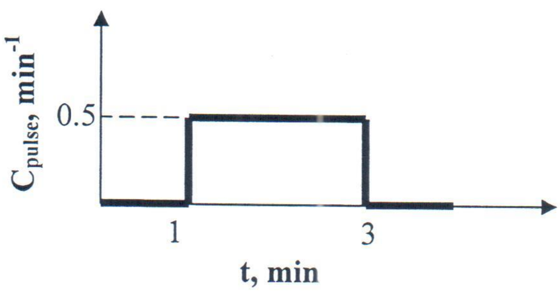
[iii] *RTD boleh digunakan untuk mengenalpasti masalah dalam reaktor. Dari plot dalam 4.[a].[i], bolehkah anda menganalisis masalah pencampuran utama dalam reaktor tangki ini?*

[3 markah]

[b] *Dalam suatu reaktor kelompok, anggapkan bahawa titisan-titisan yang tidak bergabung dan tersebar bertindak balas ketika titisan-titisan mengalir melalui suatu penyentuh. Kepekatan awal* A *ialah 2 mol/L. Maklumat tindak balas diberikan seperti berikut:*

$$A \rightarrow B,\ -r_A = kC_A^2,\ k = 0.5\ L.mol^{-1}.min^{-1}$$

[i] *Tentukan kepekatan purata* A *yang tinggal dalam titisan selepas meninggalkan penyentuh jika RTD titisan-titisan ini diberikan dalam Rajah S.4.[b].*



Rajah S.4.[b].

Petunjuk: Gunakan model terasing $(\overline{X} = \int_0^\infty X(t)E(t)dt)$. [5 markah]

[ii] *Jika tindak balas adalah tertib pertama, adakah tahap pencampuran mikro mempengaruhi penukaran purata? Ya atau tidak. Justifikasikan jawapan anda.*

[2 markah]

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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

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}[f(x_0) + f(x_1)] \text{ when } h = x_1 - x_0$$

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 $h = \dfrac{x_3 - x_0}{3}$; $x_1 = x_0 + h$; $x_2 = x_0 + 2h$;

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

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 $h = \dfrac{x_N - x_0}{N}$

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 $h = \dfrac{x_N - x_0}{N}$

Useful Integrals in Reactor Design

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

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

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

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

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

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

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

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

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

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

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

Simpson's five-point formula

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