UNIVERSITI SAINS MALAYSIA

First Semester Examination
2015/2016 Academic Session

December 2015 / January 2016

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

Duration : 3 hours
[Masa : 3 jam]

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

[Sila pastikan bahawa kertas peperiksaan ini mengandungi TUJUH muka surat yang bercetak dan SATU 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] [i] The general mole balance equation for the batch and flow reactors is given as follow:

$$F_{j0} - F_j + \int_0^V r_j dV = \frac{dN_j}{dt}$$

Convert the general mole balance equation for a given species, to a general mass balance equation of that species.

[5 marks]

[ii] The following liquid phase reaction is elementary.

$$A + 2B \rightarrow C$$

Use the equation above to explain the power law model.

[5 marks]

[b] The following reaction $A \rightarrow B$ is carried out in the following reactor scheme in Figure Q.1.[b] and the following data are recorded:

Table Q.1.[b]

X	0.0	0.2	0.4	0.6	0.65
$-r_A$ (kmol/m^3.h)	39	53	59	38	25

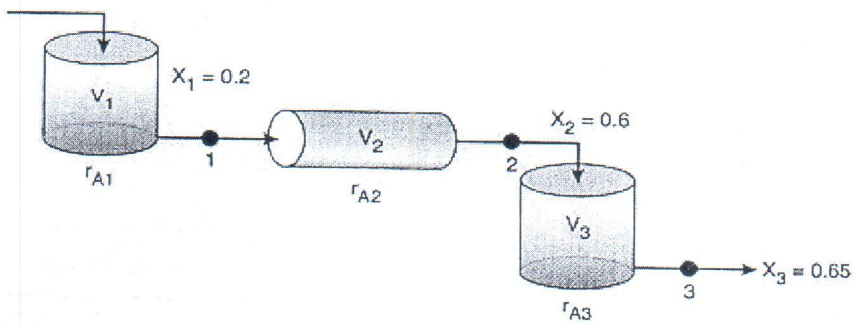


Figure Q.1.[b]. Reactors in series

[i] Use appropriate design equations to determine the volume of each of the reactors for an entering molar flow of *A* of 50 kmol/h.

[6 marks]

[ii] Process the data accordingly and construct a Levenspiel plot. Shade and label the area under curve of the respective reactors, accordingly.

[4 marks]

Jawab SEMUA soalan.

1. [a] [i] *Persamaan umum keseimbangan mol untuk reaktor-reaktor berkelompok dan aliran diberikan seperti berikut:*

$$F_{j0} - F_j + \int_0^V r_j dV = \frac{dN_j}{dt}$$

Tukar persamaan umum keseimbangan mol untuk suatu spesis kepada persamaan umum keseimbangan jisim untuk spesis tersebut.

[5 markah]

[ii] *Tindak balas fasa cecair berikut adalah asas.*

$$A + 2B \rightarrow C$$

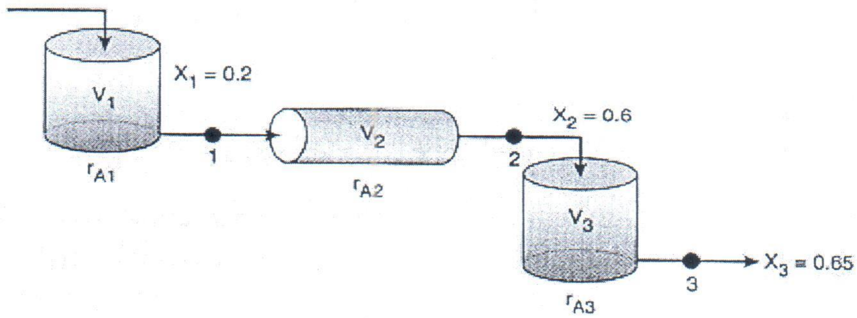
Guna persamaan tersebut untuk menerangkan model hukum kadar.

[5 markah]

[b] *Tindak balas* A → B *berikut dijalankan di dalam skim reaktor seperti dalam Gambarajah S.1.[b] dan data berikut telah direkod.*

Jadual S.1.[b]

X	0.0	0.2	0.4	0.6	0.65
$-r_A$ *(kmol/m³.j)*	39	53	59	38	25



Gambarajah S.1.[b]Reaktor Sesiri

[i] *Gunakan persamaan rekabentuk yang sesuai untuk menentukan isipadu setiap reaktor untuk aliran molar masuk A, 50 kmol/j.*

[6 markah]

[ii] *Proses data tersebut dan bina plot Levenspiel. Lorek dan label luas di bawah graf reaktor-reaktor tersebut.*

[4 markah]

[iii] Calculate the volume of reactor 3 if the reaction is carried out in a PFR reactor. Compare the value with the reactor 3 CSTR volume obtained in Q.1.[b].[i]. Justify why such difference occurred.

[5 marks]

2. [a] Using the equation of state for the gas phase, show the volume, V as a function of the conversion, X for the batch reactors with variable volume.

[5 marks]

[b] Consider the reaction $2C_4H_6 \rightarrow C_8H_{12}$ using the data in Table Q.2.[b]:

[i] Is the reaction first or second order? Plot the two graphs separately.

[10 marks]

[ii] What is the value of the rate constant for the reaction?

[5 marks]

[iii] What is the half-life for the reaction under the conditions of this experiment?

[5 marks]

Table Q.2.[b]

$[C_4H_6]$ (mol)	Time (sec)
0.0100	0
0.00625	1000
0.00476	1800
0.00370	2800
0.00313	3600
0.00270	4400
0.00241	5200
0.00208	6200

3. [a] Consider the reactions

$$A \rightarrow B, \; r_1 = k_1 = 9$$
$$A \rightarrow C, \; r_2 = k_2 C_A = 6C_A$$
$$A \rightarrow C, \; r_3 = k_3 C_A^2 = C_A^2$$

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

[i] Determine the maximum selectivity to form C.

[10 marks]

[ii] What conversion will give the maximum selectivity to C for $C_{A0} = 2\ mol.L^{-1}$?

[2 marks]

[iii] If you are the design engineer, do you recommend *PFR* or *CSTR* reactor? Justify your recommendation.

[3 marks]

[iii] *Kira isipadu reaktor 3 sekiranya tindak balas dijalankan di dalam reaktor PFR. Bandingkan nilai yang diperolehi dengan isipadu reaktor 3 CSTR dalam S.1.[b].[i]. Jelaskan mengapa perbezaan tersebut berlaku.*

[5 markah]

2. [a] *Menggunakan persamaan keadaan untuk fasa gas, tunjukkan isipadu* V *sebagai fungsi untuk pertukaran,* X *bagi reaktor berkelompok berbilang isipadu.*

[5 markah]

[b] *Ambilkira tindak balas* $2C_4H_6 \rightarrow C_8H_{12}$ *menggunakan data dalam Jadual S.2.[b].*

[i] *Adakah tindak balas tersebut tertib pertama atau kedua? Plotkan kedua-dua geraf secara berasingan.*

[10 markah]

[ii] *Apakah nilai pemalar kadar tindak balas?*

[5 markah]

[iii] *Apakah separuh-hayat untuk tindak balas mengikut keadaan eksperimen tersebut?*

[5 markah]

Jadual S.2.[b].

$[C_4H_6]$ (*mol*)	*Masa* (*saat*)
0.0100	0
0.00625	1000
0.00476	1800
0.00370	2800
0.00313	3600
0.00270	4400
0.00241	5200
0.00208	6200

3. [a] *Pertimbangkan tindak balas-tindak balas*

$A \rightarrow B,\ r_1 = k_1 = 9$
$A \rightarrow C,\ r_2 = k_2C_A = 6C_A$
$A \rightarrow C,\ r_2 = k_2C_A^2 = C_A^2$

di mana kadar dalam $mol.L^{-1}.min^{-1}$ *dan kepekatan dalam* $mol.L^{-1}$.

[i] *Tentukan pemilihan maksimum untuk membentuk C.*

[10 markah]

[ii] *Apakah penukaran yang akan memberikan pemilihan maksimum kepada* C *untuk* $C_{A0} = 2\ mol.L^{-1}$?

[2 markah]

[iii] *Sekiranya kamu jurutera rekabentuk, adakah anda mengesyorkan reaktor* PFR *atau* CSTR. *Jelaskan cadangan anda.*

[3 markah]

[b] A continuous response to a pulse injected into a reactor is summarized in Table Q.3.[b].

Table Q.3.[b]

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 exit age distribution or the residence-time distribution *(RTD)* function, *E(t)*.

[8 marks]

[ii] Calculate the mean residence time of fluid in the reactor.

[2 marks]

4. [a] For an adiabatic reactor, a reaction ($A \rightarrow B;\ r = k\ (T)\ C_A$) in aqueous phase with ΔH_R = - 104.645 kJ/mole, C_p = 4.2 J.g^{-1}.K^{-1} was conducted. The energy balance for this adiabatic reactor can be further simplified into

$$T = T_0 + \frac{(-\Delta H_R)C_{A0}X}{\rho Cp}$$

[i] Calculate the highest initial concentration of *A* (C_{A0}) to prevent boiling if the initial temperature is 300 K?

[8 marks]

[ii] Justify your answer in Q.4.[a].[i] is universally true for different types of reactor.

[4 marks]

[iii] Determine the volume of *CSTR* for 50 % conversion of this reaction if the k at 300 K is 0.2 min^{-1} and the activation energy is 125.574 kJ/mole. The initial concentration of *A* (C_{A0}) is 2 mol.L^{-1} and F_{A0} = 100 mol.min^{-1}.

[8 marks]

[b] The performance of a continuous flow reactor depends on the flow and mixing patterns to a great extent.

[i] List two factors that cause the real reactor to deviate from ideal flow patterns.

[2 marks]

[ii] A tracer is injected at the inlet of a reactor with a volume of 1100 L and a flow rate of 340 L/min. The mean residence time calculated from the truncated tracer response is $\bar{t}_E$ = 2.5 min. Estimate the percentage of the reactor volume which is considered as stagnant.

[3 marks]

[b] *Respon berterusan kepada denyutan yang disuntik ke dalam reaktor dirumuskan dalam Jadual S.3.[b].*

Jadual S.3.[b].

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

[i] *Jadual dan lakar taburan umur keluar atau fungsi agihan masa mastautin* (RTD), E (t).

[8 markah]

[ii] *Kira masa mastautin purata bendalir dalam reaktor.*

[2 markah]

4. [a] *Satu tindak balas* ($A \rightarrow B$; $r = k(T)\, CA$) *untuk reaktor adiabatik telah dijalankan dalam fasa berair* $\Delta H_R = -104.645$ *kJ/mol,* $C_p = 4.2\ J.g^{-1}.K^{-1}$ *telah dijalankan. Imbangan tenaga untuk reaktor adiabatik ini boleh diringkaskan lagi kepada*

$$T = T_0 + \frac{(-\Delta H_R)C_{A0}X}{\rho Cp}$$

[i] *Kira kepekatan awal tertinggi* A (C_{A0}) *untuk mencegah pendidihan sekiranya suhu awal adalah 300 K.*

[8 markah]

[ii] *Jelaskan jawapan anda dalam S.4.[a].[i] adalah benar untuk pelbagai jenis reaktor.*

[4 markah]

[iii] *Tentukan isipadu reaktor* CSTR *untuk penukaran 50% bagi tindak balas ini jika* k *pada 300 K adalah 0.2* min^{-1} *dan tenaga pengaktifan ialah 125.574 kJ/mol. Kepekatan awal* A (C_{A0}) *adalah 2* $mol.L^{-1}$ *dan* $F_{A0} = 100\ mol.min^{-1}$.

[8 markah]

[b] *Prestasi reaktor aliran berterusan bergantung kepada corak aliran dan percampuran pada tahap yang tinggi.*

[i] *Senarai 2 faktor yang menyebabkan reaktor sebenar menyimpang daripada corak aliran unggul.*

[2 markah]

[ii] *Penyurih* A *disuntik pada aliran masuk ke suatu reaktor yang berisipadu 1100 L dan berkadar aliran 340 L/min. Masa mastautin purata dikira daripada resapan penyurih terpangkas adalah* $\bar{t}_E = 2.5$ *min. Anggar peratusan isipadu reaktor yang dianggap sebagai bertakung.*

[3 markah]

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Appendix

Useful Equations

$$E(t) = \frac{C(t)}{\int_0^\infty C(t)dt}$$

$$E(t) = \frac{d}{dt}\left[\frac{C(t)}{C_0}\right]$$

$$t_m = \int_0^\infty tE(t)dt$$

$$\sigma^2 = \int_0^\infty (t - t_m)^2 E(t)dt$$