
UNIVERSITI SAINS MALAYSIA

First Semester Examination
2011/2012 Academic Session

January 2012

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 THREE pages of Appendix before you begin the examination.

[Sila pastikan bahawa kertas peperiksaan ini mengandungi TUJUH 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.

Jawab SEMUA soalan.

1. [a] Table Q.1.[a]. shows the kinetic data obtained for a specific reaction carried out isothermally. Using an initial concentration and volumetric flow rate for reactant A of 0.2 mol/dm³ and 0.02 m³/s respectively, answer the following questions:

Jadual S.1.[a]. menunjukkan data kinetik yang didapati bagi sesuatu tindak balas yang dijalankan pada suhu yang tetap. Dengan menggunakan kepekatan dan kadar aliran isipadu awal bagi bahan tindak balas A sebagai 0.2 mol/dm³ dan 0.02 m³/saat masing-masing, jawab soalan-soalan berikut:

Table Q.1.[a]
Jadual S.1.[a]

Conversion <i>Penukaran</i> (X)	0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
Rate of reaction, -r _A <i>Kadar tindak balas, -r_A</i> (mol/m ³ .s)	0.0667	0.1	0.138	0.2	0.222	0.235	0.2	0.174	0.138	0.0889

- [i] What is the volume of reactor and space time required to achieve 80% conversion in a Plug Flow Reactor (PFR)?

Apakah isipadu reaktor dan masa ruang yang diperlukan bagi mencapai 80% penukaran di dalam Reaktor Aliran Palam (PFR)?

[4 marks/markah]

Simpson's one-third rule for evaluating integral is given as:

Peraturan Simpson satu pertiga bagi menilai kamiran adalah diberi sebagai:

$$\int_{X_0}^{X_2} f(X) dX = \frac{h}{3} [f(X_0) + 4f(X_1) + f(X_2)]$$

where

$$h = \frac{X_2 - X_0}{2} \quad X_1 = X_0 + h$$

- [ii] Plot the concentration profile for reactant A along the reactor using the volume obtained in 1.[a].[i]. Assume that the diameter of the reactor is 1 m and only reactant A enters the reactor. State all assumptions required to plot the concentration profile, if any.

Plotkan profil kepekatan bahan tindak balas A sepanjang reaktor bagi isipadu reaktor yang didapati dalam 1.[a].[i]. Anggap diameter reaktor adalah 1 m dan hanya bahan tindak balas A memasuki reaktor. Nyatakan semua andaian yang diperlukan untuk memplot profil kepekatan.

[5 marks/markah]

- [iii] Assuming the reaction shown in Table Q.1.[a] is carried out in a Continuous Stirred Tank Reactor (CSTR) and Plug Flow Reactor with equal volume, how should they be arranged if you want to minimize the reactor volume and still achieve 80% conversion? What is the volume of the reactor? Comment on your answer.

Seandainya anda mahu menjalankan tindak balas yang ditunjukkan dalam Jadual S.1.[a]. di dalam Reaktor Tangki Campuran Berterusan dan Reaktor Aliran Palam yang mempunyai isipadu yang sama, bagaimanakah kedua-dua reaktor tersebut harus disusun untuk meminimumkan isipadu reaktor tetapi masih mencapai penukaran 80%. Apakah isipadu reaktor tersebut? Komen jawapan anda.

[10 marks/markah]

- [b] Calculate the equilibrium conversion and concentration for a liquid-phase reaction:

Kirakan kepekatan dan penukaran pada keadaan keseimbangan bagi suatu tindak balas fasa cecair berikut:



with $C_{A0} = C_{B0} = 2 \text{ mol/dm}^3$ and $K_C = 10 \text{ dm}^3/\text{mol}$.
dengan $C_{A0} = C_{B0} = 2 \text{ mol/dm}^3$ dan $K_C = 10 \text{ dm}^3/\text{mol}$.

[6 marks/markah]

2. [a] Define the following terms:
Berikan definisi istilah berikut:

[i] Elementary reaction
Tindak balas asas

[ii] Rate law
Hukum kadar

[iii] Elementary rate law
Hukum kadar asas

[6 marks/markah]

- [b] The data shown in Table Q.2.[b] were reported for a gas-phase constant volume decomposition of dimethyl ether at 504 °C in a batch reactor. Initially only (CH₃)₂O was present. The decomposition reaction can be assumed:

Data dalam Jadual S.2.[b]. adalah bagi suatu tindak balas fasa gas isipadu tetap bagi penguraian dimetil eter pada 504 °C di dalam reaktor kelompok. Pada awalnya hanya (CH₃)₂O yang wujud. Tindak balas penguraian boleh dianggap sebagai:



Also assume it is an irreversible reaction and goes to completion.
Anda juga boleh anggap ia adalah tindak balas tidak berbalik dan bertindak balas sehingga lengkap.

Table Q.2.[b]
Jadual S.2.[b].

Time (s) <i>Masa (s)</i>	390	777	1195	3155	∞
Total Pressure (mmHg) <i>Jumlah Tekanan (mmHg)</i>	408	488	562	799	931

- [i] Why do you think the total pressure measurement at t = 0 is missing? Can you estimate it?
Mengapa penyukatan jumlah tekanan pada t = 0 tidak diberikan? Bolehkah anda menganggarkan nilai tersebut?
[4 marks/markah]
- [ii] Determine the reaction order and specific reaction rate constant.
Tentukan tertib tindak balas dan pemalar kadar tindak balas spesifik.
[12 marks/markah]

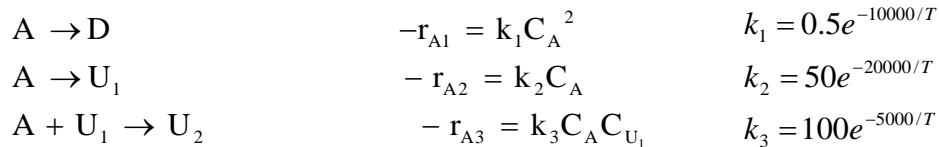
The following integral evaluation maybe useful:
Penilaian pengamiran berikut mungkin akan diperlukan:

$$\int_{P_0}^P \frac{dP}{[1 + \epsilon]P_0 - P} = \ln \left[\frac{\epsilon P_0}{(1 + \epsilon)P_0 - P} \right]$$

- [iii] How would the data shown in Table Q.2.[b] and your answers change if the reaction were run at a higher or lower temperature?
Bagaimanakah data yang diberikan dalam Jadual S.2.[b]. dan jawapan anda akan berubah sekiranya tindak balas dijalankan pada suhu yang lebih tinggi atau lebih rendah?
[3 marks/markah]

3. [a] Parallel reactions with below details (where T is expressed in K) produce desired product, D. However, U₁ and U₂ are also produced as pollutants.

Tindak balas selari dengan butiran di bawah (di mana T dinyatakan dalam K) menghasilkan produk yang dikehendaki, D. Walau bagaimanapun, U₁ dan U₂ dihasilkan sebagai bahan pencemar.



- [i] Express the instantaneous selectivity of D with respect to the pollutants U₁ and U₂ using terms, C_A and T only.

Nyatakan pemilihan serta-merta D berkenaan dengan bahan pencemar U₁ dan U₂ dengan menggunakan terma-terma C_A dan T sahaja.

[6 marks/markah]

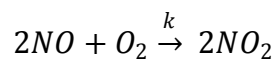
- [ii] In order to maximize the production of D, how the parallel reactions should be carried out?

Untuk memaksimumkan pengeluaran D, bagaimanakah tindak balas selari perlu dijalankan.

[4 marks/markah]

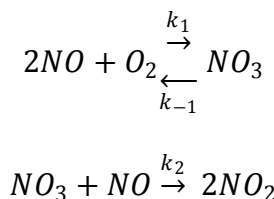
- [b] Nitrogen monoxide (NO) is oxidized into nitrogen dioxide (NO₂) with third order kinetics and an apparent negative activation energy.

Nitrogen monoksida (NO) dioksidakan kepada nitrogen dioksida (NO₂) dengan kinetik tertib ketiga dan tenaga pengaktifan negatif yang ketara.



Consider the following mechanism, in which NO₃ is an active intermediate, prove that the reaction is elementary and the rate constant k decreases with increasing temperature.

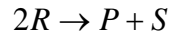
Pertimbangkan mekanisma yang berikut, di mana NO₃ ialah perantaraan aktif, buktikan bahawa tindak balas ialah tindak balas asas dan pemalar kadar k berkurang dengan penambahan suhu.



[7 marks/markah]

- [c] In a CSTR, component R reacted into P and S following in a second order reaction as shown below.

Dalam suatu CSTR, komponen R ditukarkan kepada P dan S melalui tindak balas tertib kedua seperti yang ditunjukkan di bawah.



The reaction is carried in liquid phase. The residence time distribution function for the reactor is given in Table Q.4.[b].

Tindak balas dijalankan dalam fasa cecair. Fungsi taburan masa kediaman untuk reaktor ini diberikan dalam Jadual S.4.[b].:

Table Q.4.[b].
Jadual S.4.[b].

t (s)	0	5	10	15	20	25	30	35
E(t) (s ⁻¹)	0	0	0	0.005	0.10	0.005	0	0

The entering concentration is 2 molar and the specific reaction rate is 0.06 dm³/mol.

Kepekatan suapan ialah 2 molar dan pemalar kadar tindak balas spesifik ialah 0.06 dm³/mol.

- [i] Determine the mean residence time.
Tentukan masa kediaman purata.

- [ii] Calculate the conversion would be achieved in a CSTR.
Kirakan penukaran yang boleh dicapai dalam suatu CSTR.

[8 marks/markah]

4. [a] A is isomerized adiabatically into B ($A \leftrightarrow B$) in a plug flow reactor. Under high pressure, a liquid catalyst helps to achieve a specific reaction rate of 31.1 h^{-1} at 360K. The feed is a mixture of 90mol% A and 10mol% C which is an inert. The feed enters at 330K. Calculate the reactor volume to process 163 kmol/h of feed at 60% conversion.

A diisomerkan secara adiabatik ke B ($A \leftrightarrow B$) dalam reaktor aliran palam. Di bawah tekanan tinggi, pemangkin cecair membantu untuk mencapai kadar tindak balas tertentu 31.1 j^{-1} pada 360K. Suapan ialah campuran 90 mol% A dan 10 mol% C yang lengai. Suapan masuk pada 330K. Kirakan isipadu reaktor untuk memproses 163 kmol/j suapan pada penukaran 60%.

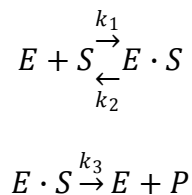
Table Q.4.[a]
Jadual S.4.[a].

Parameters	
H_{Rx}^o (273) (kJ/mol A)	-6.9
E (kJ/mol)	65.7
C_{pA} (J/mol.K)	141
C_{pB} (J/mol.K)	141
C_{pC} (J/mol.K)	161
K_c (330K) ($\text{dm}^3/\text{mol.s}$)	3.30
C_{A0} (mol/dm^3)	9.3

[20 marks/markah]

- [b] The enzymatic decomposition of S produces P using enzyme E. The reaction can be written as

Penguraian enzimatik S menghasilkan P dengan menggunakan enzim E. Tindak balas boleh ditulis sebagai



Derive an expression for the production rate of P in terms of the total enzyme concentration ($E_T = E + E \cdot S$) and S concentration using the pseudo-steady state hypothesis for the enzyme complex E·S.

Terbitkan satu ungkapan bagi kadar pengeluaran P dari segi kepekatan enzim keseluruhan ($E_T = E + E \cdot S$) dan kepekatan S menggunakan hipotesis pseudo-keadaan mantap untuk enzim kompleks E · S.

[5 marks/markah]

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-eighths rule

$$\int_{x_0}^{x_3} f(x)dx = \frac{3}{8}h[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)]$$

$$\text{Where } h = \frac{x_3 - x_0}{3}; \quad x_1 = x_0 + h; \quad x_2 = x_0 + 2h;$$

3. Simpson's quadrature formula

$$\int_{x_0}^{x_4} f(x)dx = \frac{h}{3}[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + f(x_4)]$$

$$\text{Where } h = \frac{x_4 - x_0}{4}$$

4. For N+1 points, where (N/3) is an integer,

$$\int_{x_0}^{x_N} f(x)dx = \frac{3}{8}h[f(x_0) + 3f(x_1) + 3f(x_2) + 2f(x_3) + 3f(x_4) + 3f(x_5) + \dots + 3f(x_{N-1}) + f(x_N)]$$

$$\text{Where } h = \frac{x_N - x_0}{N}$$

5. For N+1 points, where N is even,

$$\int_{x_0}^{x_N} f(x)dx = \frac{h}{3}[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \dots + 4f(x_{N-1}) + f(x_N)]$$

$$\text{Where } h = \frac{x_N - x_0}{N}$$

Ideal gas constant

$$R = \frac{8.314 \text{ kPa} \cdot \text{dm}^3}{\text{mol} \cdot \text{K}}$$

$$R = \frac{1.987 \text{ Btu}}{\text{lb mol} \cdot ^\circ \text{R}}$$

$$R = \frac{0.73 \text{ ft}^3 \cdot \text{atm}}{\text{lb mol} \cdot ^\circ \text{R}}$$

$$R = \frac{8.3144 \text{ J}}{\text{mol} \cdot \text{K}}$$

$$R = \frac{0.082 \text{ dm}^3 \cdot \text{atm}}{\text{mol} \cdot \text{K}} = \frac{0.082 \text{ m}^3 \cdot \text{atm}}{\text{kmol} \cdot \text{K}}$$

$$R = \frac{1.987 \text{ cal}}{\text{mol} \cdot \text{K}}$$

First Point

$$\left. \frac{dC_A}{dt} \right|_{t_0} = \frac{-3C_{A0} + 4C_{A1} - C_{A2}}{2\Delta t}$$

Interior Points

$$\left. \frac{dC_A}{dt} \right|_{t_i} = \frac{C_{A(i+1)} - C_{A(i-1)}}{2\Delta t}$$

Last point

$$\left. \frac{dC_A}{dt} \right|_{t_n} = \frac{C_{A(n-2)} - 4C_{A(n-1)} + 3C_{A(n)}}{2\Delta t}$$

Energy balance:

$$T = T_0 + \frac{X[-\Delta H_{Rx}(T_0)]}{\sum \phi_i \tilde{C}_{Pi} + X\Delta \tilde{C}_P}$$

Rate law:

$$k(T) = k(T_1) e^{\left[\frac{E}{R} \left(\frac{1}{T_1} - \frac{1}{T} \right) \right]}$$

Useful Integrals in Reactor Design

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

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

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

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

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

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

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

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

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

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

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

Simpson's five-point formula

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