UNIVERSITI SAINS MALAYSIA

Second Semester Examination
2010/2011 Academic Session

April/May 2011

EKC 337 – Reactor Design and Analysis
[Rekabentuk Dan Analisis Reaktor]

Duration : 3 hours
[Masa : 3 jam]

Please ensure that this examination paper contains SEVEN printed pages before you begin the examination.

[Sila pastikan bahawa kertas peperiksaan ini mengandungi TUJUH muka surat yang bercetak sebelum anda memulakan peperiksaan ini.]

Instruction: Answer **ALL** questions.

*[**Arahan:** Jawab **SEMUA** soalan.]*

In the event of any discrepancies, the English version shall be used.

[Sekiranya terdapat sebarang percanggahan pada soalan peperiksaan, versi Bahasa Inggeris hendaklah digunapakai].

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1. [a] Define the following terms:
Berikan definisi untuk istilah-istilah yang berikut:

[i] Turnover frequency
Frekuensi pusingan balik

[ii] Dispersion of the active component on the catalyst
Serakan komponen aktif pada mangkin

[4 marks/markah]

[b] List down the differences between physisorption and chemisorption.
Senaraikan perbezaan antara fizierapan dan kimierapan.

[4 marks/markah]

[c] The reaction of steam reforming of methane over a catalyst is:
Tindak balas pembentukan semula stim metana di atas mangkin,

$$CH_4 + H_2O \rightarrow CO + 3H_2$$

Propose a mechanism where the rate limiting step is the reaction between C•S and O•S, where S is the active site of the catalyst.
Cadangkan suatu mekanisma di mana langkah penghadan kadar ialah tindak balas antara C•S dan O•S, di mana S ialah tapak aktif mangkin.

[7 marks/markah]

[d] The methanol synthesis reaction
Tindak balas sintesis metanol

$$CO + 2H_2 \leftrightarrow CH_3\,OH$$

is reversible at typical operating conditions. With certain heterogeneous catalysts, the reaction is thought to proceed according to the following sequence of elementary reactions:

adalah berbalik pada keadaan operasi lazim. Dengan mangkin-mangkin heterogen tertentu, tindak balas tersebut difikirkan sebagai menuruti jujukan tindak balas-tindak balas asas yang berikut:

$CO + S^* \leftrightarrow CO–S^*$	(1)
$H_2 + S^* \leftrightarrow H_2–S^*$	(2)
$H_2–S^* + CO–S^* \leftrightarrow CH_2O–S^* + S^*$	(3)
$CH_2O–S^* + H_2–S^* \leftrightarrow CH_3OH–S^*$	(4)
$CH_3OH–S^* \leftrightarrow CH_3OH + S^*$	(5)

where *S** is an empty site on the catalyst surface, and *A–S** is species "A" adsorbed on a site. Reaction (3) is believed to be the rate-limiting step. Derive the form of the rate equation for methanol formation for this mechanism.

di mana S ialah suatu tapak kosong pada permukaan mangkin, dan A–S* ialah spesis "A" yang terjerap pada tapak. Tindak balas (3) dipercayai menjadi langkah penghadan kadar. Terbitkan bentuk persamaan kadar untuk pembentukan metanol bagi mekanisma ini.*

[10 marks/markah]

2. [a] Ammonia is produced in a process known as the Haber process, in which nitrogen and hydrogen react in the presence of an iron catalyst to form ammonia. Commercial catalysts for this process are available, but there is also opportunity to design a better catalyst. Briefly discuss possible improvements to be done towards achieving the objectives of producing high performance catalysts for this chemical reaction.

Amonia dihasilkan dalam suatu proses yang dikenali sebagai proses Haber di mana nitrogen dan hidrogen bertindak balas dengan kehadiran mangkin besi untuk membentuk amonia. Mangkin komersil boleh diperolehi namun masih terdapat peluang untuk merekabentuk mangkin yang lebih baik. Bincangkan secara ringkas pembaharuan yang boleh dilakukan untuk mencapai objektif untuk menghasilkan mangkin berprestasi tinggi untuk tindak balas ini.

[5 marks/markah]

[b] Despite producing catalysts with good metal dispersion, catalyst preparation method through ion-exchange process has several drawbacks. Provide your arguments to support this statement.

Walaupun menghasilan mangkin dengan penyerakan logam yang baik, kaedah penyediaan mangkin secara penukaran ion mempunyai beberapa kekurangan. Berikan hujah-hujah anda untuk menyokong kenyataan ini.

[5 marks/markah]

[c] A very fast reaction occurs on the external surface of a non-porous spherical catalyst pellet, 1.2 cm in diameter that is suspended in a large body of dilute liquid reactant A. When the free-system liquid velocity is increased, corresponding increase in the rate of surface reaction is detected to suggest an external mass transfer phenomenon. Given that the bulk concentration of the reactant is 1.0 M, kinematic viscosity is 0.6 centistoke (1 centistoke = 10^{-6} m^2/s) and the liquid diffusivity of A is 1.2 x 10^{-10} m^2/s. Calculate the free-system liquid velocity to be used to achieve a reaction rate per unit catalyst surface area of 0.0046 mol/(m^2.s).

Suatu tindak balas yang amat cepat berlaku pada permukaan luar pelet mangkin sfera tak berliang dengan diameter 1.2 sm yang terampai dalam bahan tindak balas cecair A yang cair. Apabila halaju bebas cecair ditingkatkan, peningkatan dalam kadar tindak balas permukaan dikesan untuk menunjukkan fenomena pemindahan jisim luaran. Diberi bahawa kepekatan pukal bahan tindak balas ialah 1.0 M, kelikatan kinematik ialah 0.6 sentistoke (1 sentistoke = 10^{-6} m^2/s) dan keresapan cecair ialah 1.2 x 10^{-10} m^2/s. Kirakan halaju bebas cecair yang perlu digunakan untuk mencapai kadar tindak balas per unit permukaan mangkin sebanyak 0.0046 mol/(m^2.s).

[7 marks/markah]

[d] In the measurement of surface area of a Ni/γ-alumina catalyst to be used for steam reforming of methane, the following nitrogen (N_2) adsorption data are obtained.

Dalam pengukuran luas permukaan mangkin Ni/γ-alumina yang perlu digunakan untuk penjelmaan stim bagi metana, data penjerapan nitrogen (N_2) berikut diperolehi.

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

$X = P/P_o$	$V(cm^3)$
0.0493	39.70
0.0789	43.62
0.1091	47.06
0.1382	50.17
0.1678	53.22
0.1978	56.28
0.2429	60.98
0.2832	65.46
0.3265	70.69
0.3235	70.04
0.2794	64.75
0.2426	60.69
0.2017	56.39
0.1709	53.25
0.1408	50.16

(Take $N_{Avogadro}$ = 6.023 x 10^{23} molecules/mole and each nitrogen (N_2) molecule occupies 0.162 nm^2). Useful equation with usual symbols;

(Ambil $N_{Avogadro}$ = 6.023 x 10^{23} molekul/mol dan setiap molekul nitrogen (N_2) menduduki 0.162 nm^2). Persamaan yang berguna dengan simbol-simbol biasa ialah:

$$\frac{x}{V(1-x)} = \frac{1}{cV_m} + \frac{(c-1)x}{cV_m}$$

[i] Calculate the Brunauer-Emmett-Teller (BET) specific surface area of the catalyst.

Kirakan luas permukaan spesifik Brunauer-Emmett-Teller (BET) bagi mangkin tersebut.

[ii] Provide two circumstances under which accurate result cannot be obtained.

Berikan dua keadaan yang boleh membuatkan keputusan yang tepat tidak dapat diperolehi.

[8 marks/markah]

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3. A palladium based monolith reactor is employed for the catalytic oxidation of 2 mol % hydrocarbon (A). Under the condition of operation, i.e. excess air, the reaction follows pseudo first-order kinetics, such that the intrinsic rate of consumption of A is given by;

Suatu reaktor monolit berasaskan paladium digunakan bagi proses pengoksidaan bermangkin 2 mol % hidrokarbon (A). Di bawah keadaan operasi, iaitu udara lebihan, tindak balas kinetik pseduo tertib-pertama, dimana kadar penggunaan hakiki komponen A diberi oleh;

$$r_A = 12 \times 10^{-6}\, p_A \text{ (mol of A/m}^2\text{.s)}$$

where p_A is the partial pressure (Pa) at the catalyst surface. The mass transfer coefficient between the bulk gas and the monolith surface is estimated as 15.2×10^{-6} mol/(m^2.Pa.s). Isothermal reactor operation is anticipated, in which temperature gradients between the gas and monolith surface are negligible.

Di mana p_A adalah tekanan separa pada permukaan mangkin (Pa). Pekali pemindahan jisim di antara gas pukal dan permukaan monolit dianggarkan sebagai 15.2×10^{-6} mol/(m^2.Pa.s). Reaktor sesuhu beroperasi diramalkan di mana kecerunan suhu di antara gas dan permukaan monolit diabaikan.

[a] Derive the overall rate equation for the reaction-diffusion process based on the bulk gas-phase partial pressure of A and determine the value of the overall rate constant.

Terbitkan persamaan kadar keseluruhan bagi proses tindak balas-resapan berasaskan tekanan separa fasa gas pukal bagi A dan tentukan nilai pemalar perkadaran keseluruhan.

[5 marks/markah]

[b] Estimate the maximum temperature difference between the gas and monolith surface, comment on the result obtained.

Anggarkan suatu nilai bagi perbezaan suhu maksimum di antara gas dan permukaan monolit, berikan komen untuk jawapan anda.

[5 marks/markah]

[c] Assuming that there is plug flow of gases through the reactor, calculate the reactor space-time required for 99% conversion of A.

Dengan mengandaikan bahawa aliran palam bagi gas-gas yang melalui reaktor, kirakan masa-ruang rektor yang diperlukan bagi 99% penukaran A.

[10 marks/markah]

[d] If the surface activity of the monolith is increased through a higher loading of palladium, such that the surface reaction is, instantaneous, calculate the reactor space-time which would then be required for 99% conversion of A.

Jika aktiviti permukaan monolit ditingkatkan melalui pertambahan muatan paladium di mana tindak balas permukaan memberi kesan serta merta, kirakan masa-ruang reaktor yang di perlukan untuk penukaran 99% A.

[5 marks/markah]

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DATA:
DATA :

Monolith area	: 85 $m^2/m^3_{reactor}$
Operating temperature	: 648 K
Gas-film heat transfer coefficient	: 2.25 kW/(m^2K)
Heat of reaction	: -170 kJ/mol
Total operational pressure	: 1 bar
Luas monolit	*: 85 $m^2/m^3_{reaktor}$*
Suhu operasi	*: 648 K*
Pekali pemindahan haba filem-gas	*: 2.25 kW/(m^2K)*
Haba tindak balas	*: -170 kJ/mol*
Tekanan operasi keseluruhan	*: 1 bar*

4. The liquid phase reaction is given by a simple reaction as follows:
Tindak balas fasa cecair diberikan oleh tindak balas ringkas seperti berikut:

$$\mathbf{A}\ (g \rightarrow l) + \mathbf{B}\ (l) \rightarrow \mathbf{P}(l)$$
$$\boldsymbol{A}\ (g \rightarrow c) + \boldsymbol{B}\ (c) \rightarrow \boldsymbol{P}(c)$$

$$r_B = 35000 C_A \text{ mol/(m}^3\text{.s)}$$

takes place in a continuous flow system in which the liquid phase may be assumed continuous and well mixed, and the gas phase dispersed (i.e. bubbles).

yang mengambil tempat di dalam sistem aliran berterusan di mana fasa cecair boleh diandaikan berterusan dan campuran sekata, serta fasa gas terserak (gelembung udara).

[a] Write down the general material balances governing the process.
Tuliskan keseimbangan jisim am yang mengawal proses tersebut.

[5 marks/markah]

[b] Simplify the model for the case in which the reaction is completed in the liquid phase.

Ringkaskan model tersebut bagi kes di mana tindak balas selesai dalam bentuk cecair.

[4 marks/markah]

[c] Show that for spherical gas bubbles of diameter d_b, the interface area per volume of reactor, a'_v, is given by

Tunjukkan bagi gelembung-gelembung udara berbentuk sfera yang berdiameter d_b*, keluasan antara-permukaan per isipadu sebuah reaktor* a'_v *diberikan oleh*

$$a'_v = \frac{6\varepsilon_g}{d_b}$$

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where ε_g is the volume fraction of gas (bubbles) in the reactor.
di mana ε_g adalah pecahan isipadu gas (gelembung-gelembung) di dalam reaktor.

[8 marks/markah]

[d] Given the data below, calculate the volume of the reactor required for 15% conversion of B. You may assume feed of B(l) to the reactor and 5 mol % A(g), complete reaction in the liquid film and negligible mass transfer resistances in the gas film. What is the conversion of A for this case?

Di beri data di bawah, kirakan isipadu reaktor yang diperlukan bagi 15% penukaran B. Anda boleh mengandaikan suapan B(c) kepada reaktor dan 5 mol % A(g), tindak balas selesai di dalam filem cecair and rintangan pemindahan jisim diabaikan pada filem gas. Apakah penukaran A di dalam kes ini?

[8 marks/markah]

DATA:
DATA :

Enhancement factor	: E ~ γ (Hatta number)
Gas molar flow rate	: 10 mol/s
Liquid molar flow rate	: 3 mol/s
Operating pressure	: 2.5 bar
Henry's Law constant for A	: 2×10^5 Pa.m^3/mol
Diffusion coefficient of A in B	: 1.5×10^{-9} m^2/s
Liquid side mass transfer coefficient	: 1.45×10^{-4} m/s
d_b	: 0.1 m
ε_g	: 0.50

Faktor tambahan	*: E ~ γ (Nombor Hatta)*
Kadar aliran gas molar	*: 10 mol/s*
Kadar aliran cecair molar	*: 3 mol/s*
Tekanan operasi	*: 2.5 bar*
Pemalar Hukum Henry bagi A	*: 2×10^5 Pa.m^3/mol*
Pemalar resapan bagi A dalam B	*: 1.5×10^{-9} m^2/s*
Pekali sebelah cecair pemindahan jisim	*: 1.45×10^{-4} m/s*
d_b	*: 0.1 m*
ε_g	*: 0.50*

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