UNIVERSITI SAINS MALAYSIA

Second Semester Examination
2011/2012 Academic Session

June 2012

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

Duration : 3 hours
[Masa : 3 jam]

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

[Sila pastikan bahawa kertas peperiksaan ini mengandungi LAPAN 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].

Answer <u>ALL</u> questions.
Jawab <u>SEMUA</u> soalan.

1. [a] In a heterogeneous catalytic reactor system, the reaction can occur only when appreciable chemisorption occurs. Briefly discuss the role of a catalyst in promoting the rate of reaction in terms of energy level, intermediate species and chemisorption process.

Dalam suatu sistem reaktor bermangkin, tindakbalas hanya akan berlaku sekiranya jerapan kimia berlaku. Bincangkan secara ringkas peranan mangkin dalam meningkatkan kadar tindakbalas dari segi tahap tenaga, spesis perantaraan dan proses jerapan kimia.

[5 marks/markah]

[b] Discuss the differences in the operation of a reactor system for complete combustion of volatile organic compounds (VOCs) and selective catalytic reduction of nitrogen oxides (NOx).

Bincangkan perbezaan antara operasi sebuah sistem reaktor untuk pembakaran lengkap sebatian organik meruap (VOC) dan penurunan bermangkin selektif bagi oksida-oksida nitrogen (NOx).

[5 marks/markah]

[c] State approaches that can be used to minimize pressure drop across the catalyst bed.

Nyatakan pendekatan-pendekatan yang boleh diguna untuk meminimakan kejatuhan tekanan merentasi lapisan mangkin.

[5 marks/markah]

[d] *i*-Pentane is produced from *n*-pentane through an isomerization reaction catalyzed by a promoted alumina catalyst. A differential reactor is used to determine the initial rate of reaction (y) as a function of partial pressure of *n*-pentane (x) and the plot is given in Figure Q.1.[d].

i-*Pentana dihasilkan dari* n-*pentana menerusi tindakbalas isomerisasi yang dimangkinkan oleh mangkin alumina. Suatu reaktor kebezaan diguna untuk menentukan kadar tindakbalas permulaan (y) sebagai fungsi tekanan separa* n-*pentana dan plotnya diberikan dalam Rajah S.1.[d].*

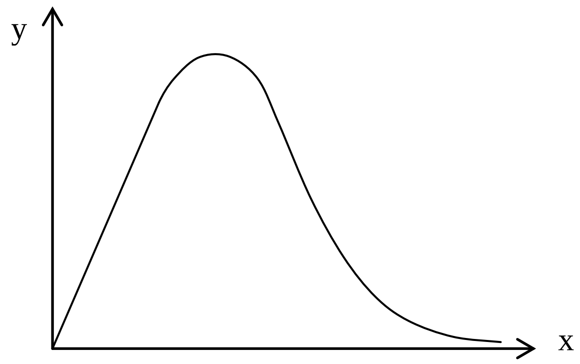

Figure Q.1.[d].
Rajah S.1.[d].

…3/-

If the conversion is known to be surface reaction-controlling, determine whether single site or dual site reaction mechanism is more appropriate to this conversion.

Sekiranya penukaran ini dihadkan oleh tindakbalas permukaan, tentukan sama ada mekanisma satu tapak atau dua tapak lebih sesuai bagi penukaran ini.

[10 marks/markah]

2. [a] Calcination of catalyst to be used in a reactor system should be performed at an optimum temperature for a suitable time. Too high temperature or too long calcination time should be avoided. Provide your argument to support this statement.

Pengkalsinan mangkin yang akan digunakan dalam sistem reaktor perlu dilakukan pada suhu optimum untuk suatu tempoh masa. Suhu yang terlampau tinggi atau tempoh pengkalsinan yang terlalu panjang patut dielakkan. Sediakan hujah-hujah anda untuk menyokong pernyataan ini.

[5 marks/markah]

[b] Shown in Figure Q.2.[b] is a typical nitrogen adsorption-desorption isotherm plot in which the hysteresis loop is observed. Explain the reasons for the different paths followed by the adsorption and desorption. If for a second catalyst material, the hysteresis loop is found to be smaller, what can be concluded on its surface characteristics as compared to the first one?

Rajah S.2.[b]. menunjukkan plot sesuhu penjerapan-penyahjerapan nitrogen di mana kelok histeresis dapat diperhatikan. Terangkan sebab-sebab mengapa laluan berlainan yang diikuti oleh proses penjerapan dan penyahjerapan. Sekiranya bagi bahan mangkin yang kedua, gelung histeresis didapati lebih kecil, apakah yang dapat disimpulkan terhadap ciri-ciri permukaannya berbanding mangkin yang pertama tadi?

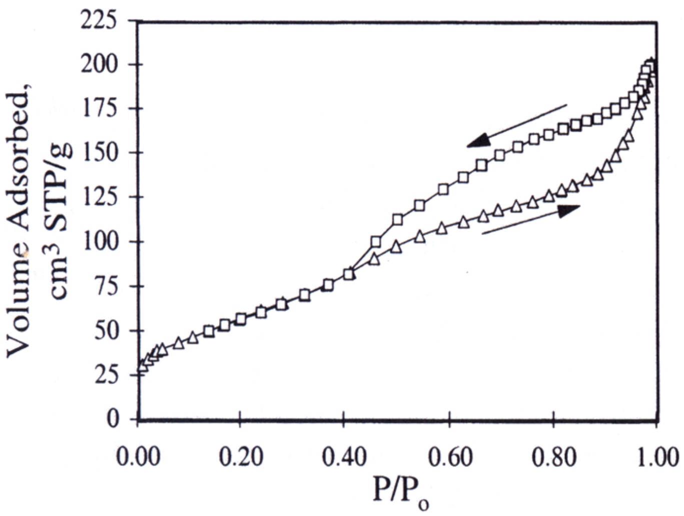

Figure Q.2.[b].
Rajah S.2.[b].

[5 marks/markah]

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[c] Temperature programmed desorption (TPD) of ammonia is a method for characterizing acidity of a catalyst material.

Kaedah penyahjerapan berprogramkan suhu (TPD) bagi amonia merupakan satu kaedah bagi pencirian keasidan bahan mangkin.

[i] Sketch a typical result that is expected to be obtained with a sample containing weak and strong acid sites.

Lakarkan keputusan lazim yang dijangka dari satu sampel yang mengandungi tapak-tapak asid lemah dan kuat.

[ii] Explain the method to be used to quantitatively measure the amount of acid sites in the catalyst sample.

Terangkan kaedah yang digunakan untuk mengukur secara kuantitatif amaun tapak asid di dalam satu sampel mangkin.

[iii] What is the main source of error in the measurement?
Apakah punca utama bagi ralat dalam pengukuran ini?

[iv] If the catalyst sample is MgO/SiO_2, sketch the expected result.
Sekiranya sampel mangkin ialah MgO/SiO_2, lakar keputusan yang dijangkakan.

[8 marks/markah]

[d] A $Fe/\gamma\text{-}Al_2O_3$ supported catalyst with 10 wt% of Fe loading in the finish catalyst is synthesized to be used for ammonia production process by reacting nitrogen with hydrogen. Incipient wetness impregnation method is used for the catalyst synthesis using 24 g of $\gamma\text{-}Al_2O_3$ and 15.0 mL of $Fe(NO_3)_2$ solution followed by drying, calcinations and reduction. Calculate the suitable concentration of metal solution to be used in the synthesis process of the supported catalyst.

Satu mangkin bersokongan $Fe/\gamma\text{-}Al_2O_3$ dengan bebanan Fe sebanyak 10 %berat dalam mangkin siap disediakan untuk proses penghasilan ammonia dengan menindakbalaskan nitrogen dan hidrogen. Kaedah impregnasi kebasahan awal digunakan untuk mensintesis mangkin menggunakan 24 g $\gamma\text{-}Al_2O_3$ dan 15.0 mL larutan $Fe(NO_3)_2$ diikuti dengan pengeringan, pengkalsinan dan penurunan. Kira kepekatan larutan logam yang sesuai diguna untuk menghasilkan mangkin tersebut.

(Atomic weight : Fe: 55.8, N: 14.0, O: 16.0)
(Berat atom : Fe: 55.8, N: 14.0, O: 16.0)

[7 marks/markah]

3. [a] According to the data given in Table Q.3.[a]., estimate the ratio of mass-transfer rates per unit volume for fixed-bed and fluidized-bed reactors at reasonable operating conditions.

Berdasarkan data yang diberi di Jadual S.3.[a]., anggarkan nisbah kadar pemindahan jisim bagi setiap unit isipadu untuk reaktor lapisan tetap dan reaktor lapisan terbendalir pada keadaan operasi yang tertentu.

Table Q.3.[a].
Jadual S.3.[a].

	Fluidized-bed *Lapisan terbendalir*	Fixed-bed *Lapisan tetap*
Particle size, d_p (cm) *Saiz zarah, d_p(sm)*	0.0063 (250 mesh)	0.635 (1/4 inch)
Void fraction of bed, ε_B *Pecahan kosong lapisan, ε_B*	0.90	0.40
Fluid mass velocity, G (g/cm^2-s) *Halaju jisim bendalir, G (g/sm^2-s)*	0.02	0.10

The general *j*-factor is given by;
Faktor-j *umum diberikan oleh:*

$$j_D = \frac{k_m \rho}{G}\left(\frac{a_m}{a_t}\right)\left(\frac{\mu}{\rho D}\right)^{\frac{2}{3}}$$

Given that, the *j*-factors are;
Diberi faktor-faktor-j*:*

- for fixed-bed reactor:
  untuk reaktor lapisan tetap:

$$j_D = \frac{0.458}{\varepsilon_B}\left(\frac{d_p G}{\mu}\right)^{-0.407}$$

- for fluidized-bed reactor:
  untuk reaktor lapisan terbendalir:

$$j_D = 1.77\left[\frac{d_p G}{\mu(1-\varepsilon_B)}\right]^{-0.44}$$

[6 marks/markah]

[b] For the catalytic oxidation of SO_2 in air, a reaction rate of 0.0956 kmol/kg-hr was measured. From the given data, calculate the temperature difference between the catalyst pellet surfaces and the bulk gas (T_{bulk} = 753 K).

Bagi pengoksidaan bermangkin SO_2 di udara, kadar tindakbalas diukur sebanyak 0.0956 kmol/kg-jam. Daripada data yang diberi, kirakan perbezaan suhu antara permukaan pelet mangkin dan gas pukal (T_{pukal} = 753 K).

<u>Data:</u>

Enthalpy change of reaction, ΔH_r:	96.37 kJ/mol
Perubahan entalpi tindakbalas, ΔH_r:	
For <u>air</u> at 753 K:	
Bagi <u>udara</u> pada 753K:	
Pr:	0.7
c_p:	1.09 kJ/kg-K
a_m:	1.05 m^2/kg
j_H:	0.31
G:	0.199 kg/m^2-s

The *j*-factor is given by:

$$j_H = \frac{\Pr^{\frac{2}{3}} h_f}{c_p G}$$

Faktor-j *diberi sebagai:*

Given an activation energy of 83.8 kJ/mol, calculate the ratio of the rate constant as measured at bulk gas temperature and surface temperature conditions. Comment on the result.

Diberi tenaga pengaktifan ialah 83.8 kJ/mol, kirakan nisbah pemalar tindakbalas yang diukur pada keadaan suhu pukal gas dan suhu permukaan. Beri pendapat anda berdasarkan keputusan yang diperolehi.

[19 marks/markah]

4. A differential reactor is used for the investigation of the catalytic decomposition of a dilute reactant described by the intrinsic kinetics.

Satu reaktor kebezaan digunakan untuk mengkaji penguraian bermangkin bahan tindakbalas cair yang diterangkan oleh kinetik hakiki

$$r_A = kC_A \qquad \text{(molA/kg-s)}$$

where C_A is the concentration of the reactant (mol/m^3). Catalyst is packed into a reactor of 0.25 ml volume and reactant fed at a rate of 1.5 μmol/s. External gas-film concentrations gradients between the pellets and the bulk gas have been determined as negligible as well as the intra-particle temperature gradients.

di mana C_A adalah kepekatan bahan tindakbalas (mol/m^3). Pemangkin dipadatkan di dalam reaktor yang berisipadu 0.25 ml dan bahan tindakbalas dialirkan pada kadar 1.5 μmol/s. Kepekatan kecerunan filem-gas luaran di antara pelet-pelet dan gas pukal telah ditentukan dan ia boleh diabaikan, begitu juga dengan kecerunan suhu di antara partikel.

In the first experiment, 0.2 g of catalyst of 80 μm mean diameter and 30.5 m^2 external surface area per kg were employed for which a conversion of 4% was measured. In a second experiment involving 0.18 g catalyst of 2000 μm mean diameter and 1.05 m^2 area per kg, a conversion of 3.2% was measured. Experiments with catalyst pellets less than 80 μm size were found to yield results which were negligibly different to the first experiment. In all cases, a temperature controller was maintained at a constant exit gas temperature of 698 K.

Di dalam ujikaji pertama, 0.2 g mangkin yang berdiameter purata 80 μm dan luas permukaan luaran, 30.5 m^2 per kg diguna bagi memberi penukaran sebanyak 4%. Di dalam ujikaji kedua yang melibatkan 0.18 g mangkin yang berdiameter purata 2000 μm dan luas permukaan per kg 1.05 m^2, penukaran 3.2% telah dicapai. Ujikaji-ujikaji dengan menggunakan pelet-pelet mangkin kurang daripada 80 μm menunjukkan bahawa keputusan yang diperolehi amat berbeza daripada ujikaji yang pertama. Bagi semua kes, satu pengawal suhu diguna untuk menetapkan suhu keluar gas pada 698 K.

[a] Calculate the observed (global) rates of reaction for the experiments using 80 μm and 2000 μm catalyst pellets and the temperature of the catalyst for each case.

Kira kadar tindakbalas yang diperhatikan (sejagat) bagi ujikaji-ujikaji yang menggunakan mangkin pelet yang bersaiz 80 μm dan 2000 μm dan suhu mangkin bagi setiap kes.

[10 marks/markah]

[b] Determine a value for the intrinsic rate constant, *k*. Given the activation energy of 95 kJ/mol, calculate the intra-particle effectiveness factor for the 2000 μm particles.

Tentukan nilai bagi pemalar kadar hakiki, k. *Diberi, tenaga pengaktifan pada 95 kJ/mol, kirakan keberkesanan antara-partikel bagi partikel bersaiz 2000 μm.*

[10 marks/markah]

[c] Assuming spherical particle geometry, estimate a value for the effective intra-particle diffusion coefficient.

Anggap geometeri partikel adalah sfera, anggarkan nilai pekali resapan berkesan antara-partikel.

<u>Data</u>:

Heat of reaction:	-229.5 kJ/mol
Particle gas-film heat transfer coefficient:	
- 80 μm particles:	22.6 J/m^2-s-K
- 2000 μm particles:	6.2 J/m^2-s-K
Total feed volumetric flow rate:	1.25 ml/s
Ideal gas constant, R:	8.314 J/mol-K

$$\eta = \frac{\tanh(\phi)}{\phi}$$ (where ϕ is the Thiele Modulus generalised for any pellet geometry)

<u>Data</u>:

Haba tindakbalas:	*-229.5 kJ/mol*
Pekali pemindahan haba filem-gas:	
- partikel berukuran 80 μm:	*22.6 J/m^2-s-K*
- partikel berukuran 2000 μm:	*6.2 J/m^2-s-K*
Jumlah isipadu kadar aliran suapan:	*1.25 ml/s*
Pekali gas unggul, R:	*8.314 J/mol-K*

$$\eta = \frac{\tanh(\phi)}{\phi}$$ *(dimana ϕ adalah Modulus Thiele umum bagi semua geometri pelet)*

[5 marks/markah]

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