UNIVERSITI SAINS MALAYSIA

Second Semester Examination
2016/2017 Academic Session

June 2017

EKC 338 – Reactor Design and Analysis
[Rekabentuk Dan Analisis Reaktor]

Duration : 3 hours
[Masa : 3 jam]

Please ensure that this examination paper contains NINE printed pages and ONE printed pages of Appendix before you begin the examination.

[Sila pastikan bahawa kertas peperiksaan ini mengandungi SEMBILAN 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].

…2/-

Answer ALL questions.

1. [a] It is desired to conduct the following gas-phase reaction on zeolite based catalyst at 210 ^{o}C and atmospheric pressure in a packed-bed reactor:

$$A \rightarrow P \qquad -r_A = \frac{50C_A}{1+0.02C_A} \text{ mol/kg.h}$$

The volumetric flow rate of pure gaseous *A* (C_{Ao} = 100 mol/m^3) is 1000 m^3/h. Calculate the amount of catalyst needed in the reactor for 80% conversion of *A*. Neglect the pressure drop in the reactor.

[10 marks]

[b] For the surface-catalyzed reaction,

$$A\,(g) + B\,(g) \rightarrow C\,(g)$$

write the reaction rate equation if :

[i] Both reactants are weakly adsorbed, and product is not adsorbed.

[1 mark]

[ii] Reactant *A* is weakly adsorbed, *B* is moderately adsorbed and product is not adsorbed.

[1 mark]

[iii] Reactant *A* is molecularly adsorbed, *B* is moderately adsorbed and product is not adsorbed.

[1 mark]

[iv] Reactant *A* is molecularly adsorbed, *B* is moderately adsorbed, product is not adsorbed and when the inert gas *(I)* is used in the feed.

[1 mark]

[c] How are the catalytic reactors classified according to size, and methods of charging and discharging? Give an example for each case.

[5 marks]

[d] Scaling up of reactors is a major task for chemical engineers. If the volume of a pilot-scale Continuous Stirred Tank Rector (CSTR) to achieve conversion X_A for a first-order irreversible liquid-phase reaction is known, using the CSTR design equation, explain how these information are used to achieve the same X_A in a larger reactor.

[6 marks]

2. [a] Discuss the importance of catalyst's particle size distribution on the optimal operation of a fluidized bed reactor.

[6 marks]

Jawab <u>SEMUA</u> soalan.

1. [a] *Adalah diinginkan untuk menjalankan tindak balas fasa-gas yang berikut di atas mangkin berasaskan zeolit pada 210 ^oC dan tekanan atmosfera di dalam sebuah reaktor lapisan-terpadat :*

$$A \rightarrow P \qquad -r_A = \frac{50C_A}{1+0.02C_A} \text{ mol/kg.j}$$

Kadar aliran isipadu gas tulen A *(C_{Ao} = 100 mol/m^3) adalah 1000 m^3/j. Kirakan jumlah mangkin yang diperlukan di dalam reaktor tersebut untuk penukaran 80%* A*. Abaikan kejatuhan tekanan di dalam reaktor tersebut.*

[10 markah]

[b] *Bagi tindak balas termangkin-permukaan,*

$$A\ (g) + B\ (g) \rightarrow C\ (g)$$

Tuliskan persamaan kadar tindak balas sekiranya :

[i] *Kedua-dua bahan tindak balas terjerap secara lemah dan produk tidak dijerap.*

[1 markah]

[ii] *Bahan tindak balas* A *terjerap secara lemah,* B *terjerap secara sederhana dan produk tidak terjerap.*

[1 markah]

[iii] *Bahan tindak balas* A *terjerap secara molekul,* B *terjerap secara sederhana dan produk tidak dijerap.*

[1 markah]

[iv] *Bahan tindak balas* A *terjerap secara molekul,* B *terjerap secara sederhana, produk tidak terjerap dan bila gas lengai* (I) *telah digunakan di dalam aliran suapan.*

[1 markah]

[c] *Bagaimanakah reaktor mangkin dikelaskan mengikut saiz, dan kaedah suapan dan luahan? Berikan contoh bagi setiap kes.*

[5 markah]

[d] *Penskalaan naik reaktor adalah tugas utama bagi jurutera kimia. Jika isipadu sebuah reaktor tangki teraduk berterusan (CSTR) berskala-pandu untuk mencapai suatu penukaran* X_A *bagi tindak balas fasa-cecair tertib pertama tak berbalik diketahui, dengan menggunakan persamaan rekabentuk CSTR, terangkan bagaimana maklumat tersebut boleh digunakan untuk mencapai* X_A *yang sama di dalam reaktor yang lebih besar.*

[6 markah]

2. [a] *Bincangkan kepentingan taburan saiz partikel terhadap operasi optimum bagi sebuah reaktor lapisan terbendalir.*

[6 markah]

[b] A *Fe/SiO_2* supported catalyst with 2.4 wt. % of *Fe* content in the finished catalyst is synthesized using incipient wetness impregnation method to be used in lab-scale for ammonia synthesis from hydrogen and nitrogen. In the catalyst synthesis method, 50.0 g of SiO_2 and 20 mL of $Fe(NO_3)_2$ solution are used followed by drying, calcinations and reduction. Calculate the concentration of the metal salt solution to be used to synthesize the catalyst.

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

[5 marks]

[c] A *Pd/γ-Al_2O_3* supported catalyst is characterized for specific surface area based on nitrogen adsorption isotherm in which V_{ads} (cm^3 STP/g_{cat}) and nitrogen partial pressure (P/P_o) data are collected. When the obtained data are plotted according to the usual Brunauer-Emmett-Teller (BET) method between $0<P/P_o<0.3$, the value of *y-axis* intercept is found to be 3.96×10^{-4} and the slope for the linear line is 0.0122.

[i] Taking the surface area covered by a single N_2 molecule is 0.162 nm^2, calculate the specific surface area of the catalyst sample.

[4 marks]

[ii] After catalyst is used in the combustion of organic pollutants in air at 550 ^oC in a packed bed reactor, the surface area is found to drop by 30%. Suggest 3 mechanisms leading to the observation.

[3 marks]

[d] Biodiesel or Fatty Acid Methyl Ester (FAME) is produced through a reaction between vegetable oil (a triglyceride) and methanol as given in Figure Q.2.[d] below.

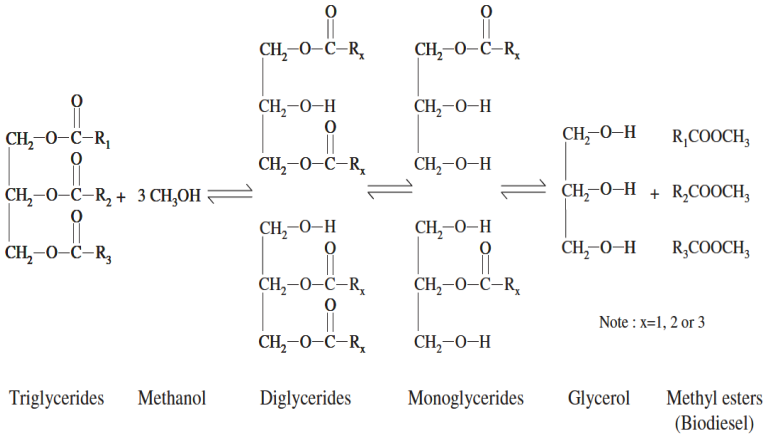


Figure Q.2.[d]

The homogeneous catalyst which is commonly used for this reaction is *NaOH*. However, currently it is being replaced by suitable solid catalysts. Justify this technological change in terms of safety, health and environmental aspects of the process.

[7 marks]

[b] *Suatu mangkin bersokongan* Fe/SiO_2 *dengan 2.4% kandungan* Fe *dalam mangkin siap disentesis menggunakan kaedah impregnasi kebasahan mula untuk sintesis ammonia skala makmal daripada hidrogen dan nitrogen. Di dalam kaedah sintesis mangkin tersebut, 50.0 g* SiO_2 *dan 20 mL* $Fe(NO_3)_2$ *digunakan diikuti dengan pengeringan, pengkalsinan dan penurunan. Kirakan kepekatan larutan garam logam tersebut yang perlu digunakan.*

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

[5 markah]

[c] *Suatu mangkin bersokongan* $Pd/\gamma\text{-}Al_2O_3$ *dicirikan untuk luas permukaan spesifik berdasarkan kaedah penjerapan nitrogen sesuhu di mana data* V_{ads} *(*sm^3 *STP/*g_{cat}*) dan tekanan separa nitrogen (*P/P_o*) diambil. Apabila data tersebut diplotkan berdasarkan kaedah Brunauer-Emmett-Teller (BET) yang biasa antara* $0<P/P_o<0.3$*, nilai pintasan paksi* y *ialah* 3.96×10^{-4} *dan kecerunan bagi garis lurus tersebut ialah 0.0122.*

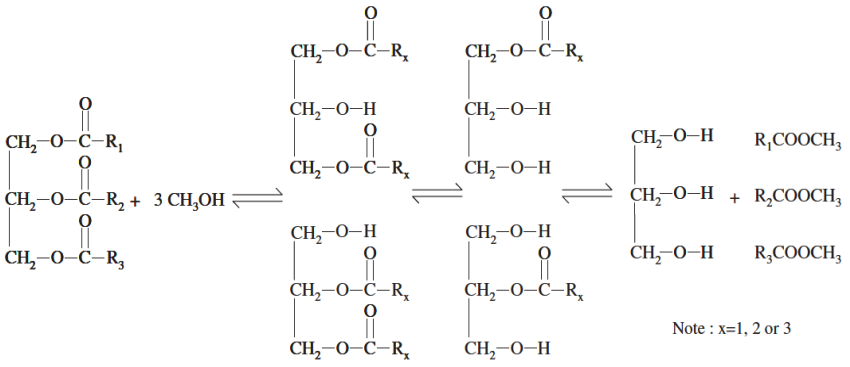
[i] *Dengan mengambil luas permukaan yang dilitupi oleh satu molekul* N_2 *ialah 0.162* nm^2*, kirakan luas permukaan spesifik bagi sampel mangkin tersebut.*

[4 markah]

[ii] *Selepas mangkin digunakan dalam pembakaran bahan cemar organik di dalam udara yang dijalankan pada 550 ℃ dalam reaktor lapisan terpadat, luas permukaan didapati menurun sebanyak 30 % . Cadangkan tiga (3) mekanisma yang menyumbang terhadap pemerhatian ini.*

[3 markah]

[d] *Biodiesel atau Metil Ester Asid Lemak* (FAME) *dihasilkan menerusi tindak balas antara minyak sayuran (trigliserida) dan metanol sebagai mana yang diberikan oleh Rajah S.2 [d] di bawah.*



Trigliserida *Metanol* *Digliserida* *Monogliserida* *Gliserol* *Ester Metil (Biodiesel)*

Rajah S.2 [d]

Mangkin homogen yang biasa digunakan untuk tindak balas ini ialah NaOH. *Bagaimanapun, ia kini digantikan dengan mangkin pepejal yang sesuai. Berikan kewajaran perubahan teknologi ini dari segi aspek keselamatan, kesihatan dan alam sekitar bagi proses tersebut.*

[7 markah]

…6/-

3. A gas oil is catalytically cracked at 903 K and 1 bar by passing vaporised feed through a differential reactor packed with spherical silica alumina pellets of radius 0.088 cm. For a feed rate of 204.5 kmol/$m^3_{reactor}$-hr, a 50% conversion is measured. The reaction can be assumed as first order and external-film mass transfer resistance is neglected. The following data are also known;

bed bulk density = 700 kg/m^3
effective diffusivity in catalyst = 8×10^{-8} m^2/s
average reactant concentration = 6.0 mol/m^3

[a] Distinguish between a differential and integral reactor.

[3 marks]

[b] Calculate the average reaction rate (in mol/kg-s) in the reactor.

[5 marks]

[c] Using the Weizs-Prater criteria, determine whether or not pore diffusion is important.

[6 marks]

[d] Calculate the intraparticle effectiveness factor, η, and the general Thiele modulus, ϕ.

[6 marks]

[e] Determine the value of the reaction rate constant.

[5 marks]

4. The parallel decomposition of a hydrocarbon is to be carried out in an isothermal fluidized bed reactor with the chemical rate equations given below;

$A \longrightarrow B$	$(r_1 = k_1 C_A)$	(mol/kg·s)
$A \longrightarrow C$	$(r_2 = k_2 C_A)$	(mol/kg·s)

Geldart classification of the catalyst particles suggests that bubble bed operation is feasible. As a preliminary design, a two-phase fluidization model is to be employed, involving the plug flow of the bubble phase. The net gas flow through the emulsion phase is predicted to be negligible. Furthermore, any reaction in the bubble phase is expected to be insignificant.

[a] Comment on the conditions at which the gas flow rate through the emulsion phase can be neglected.

[*2 marks*]

3. *Suatu minyak gas melalui proses pecahan bermangkin pada suhu 903 K dan 1 bar dengan melalukan bekalan terpelewap menerusi satu reaktor kebezaan yang dipadatkan dengan until silika alumina pada jejari 0.088 sm. Dengan kadar bekalan 204.5kmol/$m^3_{reaktor}$-jr, 50% kadar penukaran. Tindak balas boleh terukur dianggap sebagai tertib pertama dan rintangan pemindahan jisim-lapisan luar diabaikan. Data-data di bawah juga diketahui ;*

ketumpatan pukal lapisan = 700 kg/m^3
kemeresapan berkesan pada mangkin = 8 × 10^{-8} m^2/s
kepekatan purata bahan tindak balas = 6.0 mol/m^3

[a] Bezakan di antara reaktor kebezaan dan reaktor kamiran.

[3 markah]

[b] Kirakan purata kadar tindak balas (dalam mol/kg-s) dalam reaktor.

[5 markah]

[c] Dengan menggunakan kriteria Weizs-Prater, *tentukan sama ada resapan liang penting atau sebaliknya.*

[6 markah]

[d] Kirakan faktor keberkesanan intra-partikel, η, *dan modulus Thiele umum,* ϕ.

[6 markah]

[e] Tentukan nilai pemalar kadar tindak balas.

[5 markah]

4. *Penguraian hidrokarbon selari akan dilakukan dalam reaktor lapisan terbendalir isotermal dengan persamaan perkadaran kimia diberikan seperti di bawah;*

$A \longrightarrow B$	$(r_1 = k_1 C_A)$	*(mol/kg·s)*
$A \longrightarrow C$	$(r_2 = k_2 C_A)$	*(mol/kg·s)*

Klasifikasi Geldart *partikel mangkin menyatakan bahawa penggunaan lapisan gelembung boleh dilaksanakan. Sebagai rekabentuk permulaan, model terbendalir dua-fasa akan digunapakai, yang memerlukan aliran palam pada fasa gelembung. Aliran bersih gas melalui fasa emulsi diramalkan boleh diabaikan. Sebagai tambahan, mana-mana tindak balas di dalam fasa gelombang dianggap tidak signifikan.*

[a] Komen keadaan-keadaan di mana kadar aliran gas melalui fasa emulsi boleh diabaikan.

[2 markah]

[b] Using appropriate parameters, write down the material balance for the bubble phase. State any additional assumptions made in your derivation.

Model parameters:

f_b	fraction of bed occupied by bubbles
g_b	mass of solids in bubble phase (kg/m^3)
g_e	mass of solids in emulsion phase (kg/m^3)
K_I	gas interchange coefficient between bubble and emulsion phases (s^{-1})
L	length of fluidized bed (m)
u_b	bubble velocity (m/s)
u_0	feed gas velocity (m/s)

[*8 marks*]

[c] Show that at any bed position, the emulsion phase concentration of reactant (C_{Ae}) is given by;

$$C_{Ae} = \kappa C_{Ab}$$

where C_{Ab} is the bubble phase gas concentration and κ is a constant. What is the functional relationship of κ with respect to the gas interchange coefficient (K_I) and the reaction rate constants k_1 and k_2?

[*5 marks*]

[d] Show that under the conditions specified in [c] above, the conversion of *A* is given by;

$$x_A \sim 1 - e^{\left[\frac{-K_I(1-\kappa)L}{u_0}\right]}$$

[*8 marks*]

[e] How would the above expression derived in [d] change for a process which was severely limited by gas interchange between the two phases?

[*2 marks*]

[b] *Dengan menggunakan pemalar-pemalar yang bersesuaian, tuliskan imbangan jisim untuk fasa gelembung. Nyatakan anggapan tambahan di dalam terbitan anda.*

Model pemalar-pemalar :

f_b *pecahan lapisan yang dipenuhi gelembung*
g_b *jisim pepejal dalam fasa gelembung (kg/m^3)*
g_e *jisim pepejal dalam fasa emulsi (kg/m^3)*
K_I *pekali saling tukar gas di antara fasa-fasa gelembung dan emulsi (s^{-1})*
L *panjang lapisan terbendalir (m)*
u_b *halaju gelembung (m/s)*
u_0 *halaju bekalan gas (m/s)*

[8 markah]

[c] *Tunjukkan pada mana-mana posisi lapisan, kepekatan bahan tindak balas emulsi,* (C_{Ae}) *diberi sebagai ;*

$$C_{Ae} = \kappa\, C_{Ab}$$

di mana C_{Ab} *adalah kepekatan gas fasa gelembung dan* κ *adalah pemalar. Apakah fungsi perkaitan* κ *dengan pekali saling tukar gas* (K_I) *dan pemalar-pemalar kadar tindak balas* k_1 *dan* k_2*?*

[5 markah]

[d] *Tunjukkan di bawah keadaan-keadaan yang dinyatakan pada [c] di atas, kadar pertukaran* A *diberikan sebagai ;*

$$x_A \sim 1 - e^{\left[\frac{-K_I(1-\kappa)L}{u_0}\right]}$$

[8 markah]

[e] *Bagaimanakah persamaan yang diterbitkan di bahagian [d] berubah pada proses yang sangat terhad dengan saling tukar gas di antara dua fasa?*

[2 markah]

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APPENDIX

Useful Integrals in Reactor Design

$$\int_0^x \frac{dx}{1-x} = \ln \frac{1}{1-x}$$

$$\int_{x_1}^{x_2} \frac{dx}{(1-x)^2} = \frac{1}{1-x_2} - \frac{1}{1-x_1}$$

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

$$\int_0^x \frac{dx}{1+\varepsilon x} = \frac{1}{\varepsilon} \ln (1+\varepsilon x)$$

$$\int_0^x \frac{(1+ex)dx}{1-x} = (1+\varepsilon) \ln \frac{1}{1-x} - \varepsilon x$$

$$\int_0^x \frac{(1+ex)dx}{(1-x)^2} = \frac{(1+\varepsilon)x}{1-x} - \varepsilon \ln \frac{1}{1-x}$$

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

$$\int_0^x \frac{dx}{(1-x)(\Theta_B - x)} = \frac{1}{\Theta_B - 1} \ln \frac{\Theta_B - x}{\Theta_B (1-x)} \qquad \Theta_B \neq 1$$

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

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

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

where p and q are the roots of the equation.

$$ax^2 + bx + c = 0 \qquad \text{i.e., } p, q = \frac{-b \mp \sqrt{b^2-4ac}}{2a}$$

$$\int_0^x \frac{a+bx}{c+gx} dx = \frac{bx}{g} + \frac{ag-bc}{g^2} \ln \frac{c+gx}{c}$$