UNIVERSITI SAINS MALAYSIA

First Semester Examination
Academic Session 2007/2008

October/November 2007

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 TWO pages of Appendix before you begin the examination.

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

Instructions: Answer any **FOUR** (4) questions.

*[**Arahan**:Jawab mana-mana **EMPAT** (4) soalan.]*

You may answer a question either in Bahasa Malaysia or in English.

[Anda dibenarkan menjawab soalan sama ada dalam Bahasa Malaysia atau Bahasa Inggeris.]

1. [a] A plug-flow reactor (PFR) may be used for both liquid-phase and gas-phase reactions. Please state whether the following characteristics of PFR are true or false.

Reaktor aliran palam (PFR) boleh digunakan untuk kedua-dua tindakbalas fasa cecair dan gas. Sila nyatakan sama ada ciri-ciri reaktor aliran palam berikut adalah benar atau salah.

[i] The flow through the vessel, both input and output streams are continuous and at constant rate.

Kedua-dua aliran masuk dan keluar yang mengalir melalui reaktor adalah berterusan dan pada kadar malar.

[ii] The system mass inside the vessel is fixed.

Jisim sistem di dalam reaktor adalah tetap.

[iii] There is no axial mixing of fluid inside the vessel.

Tiada percampuran paksi bagi bendalir di dalam reaktor.

[iv] There is complete radial mixing if fluid inside the vessel, thus the properties of the fluid are not uniform in this plane.

Percampuran jejarian adalah sempurna jika bendalir berada di dalam reaktor. Oleh itu, ciri-ciri bendalir pada satah ini adalah tidak seragam.

[v] The density of the flowing system may vary in the direction of flow.

Ketumpatan sistem yang mengalir mungkin berubah mengikut arah aliran.

[vi] The system may operate at steady state or at unsteady state.

Sistem mungkin beroperasi pada keadaan mantap ataupun keadaan tidak mantap.

[vii] There is no heat transfer through the walls of the vessel between the system and the surroundings.

Tiada pemindahan haba menerusi dinding reaktor di antara sistem dan sekeliling.

[7 marks/markah]

[b] If you have a CSTR and a PFR (both at the same volume) available to carry out an irreversible, first order, liquid-phase reaction, how would you connect them in series (in what order) to maximize the conversion?

Bagaimana kamu menghubungkan reaktor tangki teraduk berterusan dan reaktor aliran palam (kedua-duanya mempunyai isipadu yang sama) secara siri untuk memaksimumkan penukaran jika kedua-duanya boleh digunakan untuk menjalankan tindakabalas tidak berbalik, tetib pertama dan dalam fasa cecair.

[8 marks/markah]

[c] The first order reaction of $A \rightarrow B$ occurs in (n) equal volume CSTR in series, each with residence time, τ, with 90% overall conversion. If $k = 0.5\ min^{-1}$, $C_{A_0} = 2$ moles/liter, and $\mu = 4$ liter/min, what residence times and reactor volumes will be required for n = 1 and 4?

Tindakbalas tertib pertama $A \rightarrow B$ berlaku dalam reaktor tangki teraduk berterusan secara siri yang mempunyai (n) buah isipadu yang sama. Setiap reaktor mempunyai masa mastautin, τ, dan 90% penukaran keseluruhan. Jika $k = 0.5\ min^{-1}$, $C_{A_0} = 2$ mol/liter, dan $\mu = 4$ liter/min, apakah masa mastautin dan isipadu reaktor yang diperlukan bagi n = 1 dan 4?

[10 marks/markah]

2. [a] Find the reactor volume required to obtain 90% conversion in the reaction

cari isipadu reaktor yang diperlukan untuk mendapat 90% penukaran dalam tindakbalas

$$A \rightarrow n_B B \quad , \quad r = k\,C_A$$

treating ideal gases in a PFR with no diluent for $n_B = 2$ and ½ with C_{A_0} = 2 moles/liter, $k = 0.5\ min^{-1}$ and $\nu_o = 4$ liters/min.

Anggap gas-gas unggul di dalam reaktor aliran palam tidak mempunyai bahan pencair apabila $n_B = 2$ dan ½, $C_{A_0} = 2$ mol/liter, $k = 0.5\ min^{-1}$ dan ν_o = 4 liter/min.

[10 marks/markah]

[b] A small reaction bomb is filled with pure reactant A at 1 atm pressure. The operation is carried out at 25°C. The temperature is then raised as rapidly as possible to 100°C and the results in Table Q. 2 [b] are given. After some time, the content of the bomb are analyzed for A and found that all A have been consumed. By using integral method find a rate equation in units of moles, liters and minutes which will satisfactory fit the data.

Reaktor yang kecil diisi dengan bahan tindakbalas tulen A pada tekanan 1 atm. Operasi dijalankan pada 25°C. Suhu kemudiannya dinaikkan secepat mungkin kepada 100°C dan keputusannya diberi dalam Jadual S.2.[b]. Selepas seketika, kandungan dalam reaktor dianalisa dan didapati kesemua bahan A telah digunakan. Dengan menggunakan kaedah pengamiran, cari persamaan kadar dalam unit mol, liter dan minit yang dapat memadankan data-data tersebut.

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

T, min	P_A (atm)
0	1.252
1	1.028
2	0.828
3	0.712
4	0.628
5	0.558
6	0.488
7	0.448
8	0.412
9	0.378
10	0.348
15	0.256
20	0.204

[15 marks/markah]

3. [a] A solution of A is mixed with an equal volume of a solution of B containing the same number of moles and the reaction A + B = C occurs. At the end of 1 hour, A is 75% reacted. How much of A will be left unreacted at the end of 2 hours if the reaction is:

Larutan A dan B yang masing-masing mempunyai isipadu dan bilangan mol yang sama dicampurkan dan tindakbalas A + B = C berlaku. Selepas 1 jam, 75% A telah bertindakbalas. Berapa banyak A yang masih tidak bertindakbalas selepas 2 jam, jika tindakbalas adalah:

[i] First order in A and zero order in B

Tertib pertama dalam A dan tertib sifar dalam B

[ii] First order in both A and B

Tertib pertama dalam A dan B

[iii] Zero order in both A and B

Tertib sifar dalam A dan B

[15 marks/markah]

[b] What reaction schemes and conditions would you use to maximize the selectivity parameter S for the following parallel reactions:

Apakah kaedah tindakbalas dan keadaan yang akan kamu gunakan untuk memaksimumkan pemilihan parameter S untuk tindakbalas selari yang berikut:

$$A + C \rightarrow D \qquad r_D = 800e^{\left(-\frac{2000}{T}\right)} C_A^{0.5} C_c$$

$$A + C \rightarrow U_1 \qquad r_{U} = 10e^{(-300/T)} C_A C_C$$

where D is the desired product and U_1 is the undesired product?

di mana D ialah hasil yang dikehendaki sementara U_1 ialah hasil yang tidak dikehendaki?

[10 marks/markah]

4. [a] The pyrolysis of acetaldehyde is believed to take place according to the following sequence:

Pirolisis asetaldehid adalah dipercayai berlaku dalam turutan yang berikut:

$$CH_3CHO \xrightarrow{k_1} CH_3\cdot + CHO\cdot$$

$$CH_3\cdot + CH_3CHO \xrightarrow{k_2} CH_3\cdot + CO + CH_4$$

$$CHO\cdot + CH_3CHO \xrightarrow{k_3} CH_3\cdot + 2CO + H_2$$

$$2CH_3\cdot \xrightarrow{k_4} C_2H_6$$

[i] Derive the rate expression for the rate of disappearance of acetaldehyde, $-r_{Ac}$

Terbitkan kadar tindakbalas untuk kadar kehilangan asetaldehid, $-r_{Ac}$

[ii] Under what conditions does it reduce to $-r_{CH_3CHO} = kC_{CH_3CHO}^{3/2}$

Dalam keadaan apakah ia akan menjadi $-r_{CH_3CHO} = kC_{CH_3CHO}^{3/2}$

[iii] Sketch a reaction pathway diagram for this reaction

Lakar gambarajah laluan tindakbalas untuk tindakbalas ini

[15 marks/markah]

[b] [i] Determine the equilibrium conversion for the elementary aqueous phase reaction. Between 0°C and 100°C:

$$A \Leftrightarrow R \begin{cases} \Delta G^0_{298} = -14130 \ J/mol \\ \Delta H^0_{298} = -75300 \ J/mol \end{cases} \qquad C_{pA} = C_{pR} = \text{constant}$$

Present the results in the form of a plot of temperature versus conversion.

Tentukan penukaran pada keadaan keseimbangan untuk tindakbalas asas fasa akues di antara 0°C dan 100°C yang berikut:

$$A \Leftrightarrow R \begin{cases} \Delta G^0_{298} = -14130 J/mol \\ \Delta H^0_{298} = -75300 J/mol \end{cases} \qquad C_{pA} = C_{pR} = malar$$

Tunjukkan keputusan kamu dalam bentuk graf suhu melawan penukaran.

[ii] What restrictions should be placed on the reactor operating isothermally if we are to obtain a conversion of 75% or higher?

Apakah kekangan yang perlu diletakkan ke atas reaktor yang beroperasi secara isotermal jika penukaran melebihi 75% atau lebih diperlukan?

[10 marks/markah]

5. [a] The gas-phase homogeneous oxidation of nitrogen monoxide (NO) to nitrogen dioxide (NO_2).

Tindakbalas pengoksidaan homogen fasa gas nitrogen monoksida (NO) kepada nitrogen dioksida (NO_2).

$$2NO + O_2 \xrightarrow{k} 2NO_2$$

is known to have a form of third-order kinetics which suggests that the reaction is elementary as written, at least for low partial pressures of the nitrogen oxides. However, the rate constant k actually decreases with increasing absolute temperature, indicating an apparently negative activation energy. Because the activation energy of any elementary reaction must be positive, some explanation is in order. Provide an explanation, based on suitable reaction mechanism starting from the fact that an active intermediate species, NO_3, is a participant in some other known reactions that involve oxides of nitrogen.

diketahui mempunyai kadar tindakbalas tertib ketiga untuk keadaan tekanan separa nitrogen oksida yang rendah. Walaubagaimanapun, pemalar kadar tindakbalas k bekurang dengan kenaikan suhu mutlak. Ini menunjukkan nilai tenaga pengaktifan yang negatif. Memandangkan tenaga pengaktifan biasanya bernilai positif, suatu penjelasan diperlukan. Jelaskan keadaan ini berdasar suatu mekanisma tindakbalas yang bermula daripada NO_3, iaitu bahantaraaktif yang terlibat dalam tindakbalas yang melibatkan oksida-oksida nitrogen

[10 marks/markah]

[b] An RTD analysis was carried out on a liquid-phase reactor and the following data are presented :

Satu analisa RTD telah dijalankan di dalam reaktor berfasa cecair dan data yang berikut telah diperolehi :

t(s)	0	150	175	200	225	240	250	260
C × 10^3(g/dm^3)	0	0	1	3	7.4	9.4	9.7	9.4

t(s)	275	300	325	350	375	400	450
C × 10^3(g/dm^3)	8.2	5.0	2.5	1.2	0.5	0.2	0

[i] Plot the E(t) curve for these data

Plot lengkung E(t) untuk data di atas

[ii] What fraction of the material spends between 230 and 270 s in the reactor?

Berapakah pecahan dari bahan yang berada di antara 230 dan 270 saat di dalam reaktor?

[iii] Plot the F(t) curve for these data

Plot lengkung F(t) untuk data di atas

[iv] What fraction of the material spends less than 250 s in the reactor?

Berapakah pecahan dari bahan yang berada kurang dari 250 saat di dalam reaktor?

[v] What is the mean residence time?

Berapa min masa mastautin?

[15 marks/markah]

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Lampiran

Useful Integrals in Reactor Design

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

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

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

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

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

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

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

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

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

$$\int_0^W (1-aW)^{1/2}\, dW = \frac{2}{3a}\left[1-(1-aW)^{3/2}\right] \qquad (A-10)$$

$$\int_0^\infty \left(e^{-kt}\right)\delta(t-\tau)\,dt = e^{-k\tau} \qquad (A-11)$$

Simpson's five-point formula

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