UNIVERSITI SAINS MALAYSIA

Peperiksaan Semester Pertama
Sidang Akademik 1997/98

September 1997

EKC 450 Simulasi dan Pengoptimuman Proses

Masa: [3 jam]

ARAHAN KEPADA CALON:

Sila pastikan soalan peperiksaan ini mengandungi **LAPAN (8)** mukasurat bercetak dan **TIGA (3)** Lampiran sebelum anda memulakan peperiksaan.

Kertas soalan ini mengandungi **LIMA (5)** soalan.

Jawab mana-mana **EMPAT (4)** soalan.

Satu soalan **MESTI** dijawab dalam Bahasa Malaysia.

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1. Penukaran glukosa kepada asid glukonik adalah melalui tindakbalas pengoksidaan kumpulan aldehid gula tersebut kepada kumpulan karboksil. Transformasi itu boleh dicapai dengan proses fermentasi menggunakan mikroorganisma. Kehadiran enzim glucose oxidase di dalam mikroorganisma menukarkan glukosa ke glukonolakton. Seterusnya, glukonolakton dihidrolisiskan kepada asid glukonik. Mekanisma keseluruhan proses fermentasi ini dilakukan dengan transformasi yang dikenali sebagai pertumbuhan sel.

The conversion of glucose to gluconic acid is a simple oxidation of the aldehyde group of the sugar to a carboxyl group. This transformation can be achieved by a microorganism in a fermentation process. The enzyme glucose oxidase, present in the microorganism, converts glucose to gluconolactone. In turn, the gluconolactone hydrolyzes to form the gluconic acid. The overall mechanism of the fermentation process which performs this transformation can be described as cell growth.

$$\text{Glucose} + \text{Cells} \rightarrow \text{Cells}$$

Pengoksidaan glukosa *Glucose oxidation*:

$$\text{Glucose} + O_2 \xrightarrow{\text{Glucose oxidase}} \text{gluconolactone} + H_2O$$

Hidrolisis glukonolakton *Gluconolactone hydrolysis*:

$$\text{Gluconolactone} + H_2O_2 \rightarrow \text{gluconic acid}$$

Penguraian peroksida *Peroxide decomposition*:

$$H_2O_2 \xrightarrow{\text{catalase}} H_2O + \frac{1}{2}O_2$$

Model matematik fermentasi menggunakan bakteria pseudomonas ovadis di mana ia mengeluarkan asid glukonik telah dibentuk. Model ini menerangkan fasa tumbesaran logaritma secara dinamik yang boleh dirumuskan seperti di bawah:

A mathematical model of the fermentation using the bacterium pseudomonas ovadis, which produces gluconic acid, has been developed. This model, which describes the dynamics of the logarithmic growth phase, can be summarised as follows:

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Kadar pertumbuhan sel
Rate of cell growth

$$\frac{dy_1}{dt} = b_1 y_1 \left(1.0 - \frac{y_1}{b_2}\right)$$

Kadar pembentukan glukonolakton:
Rate of gluconolactone formation:

$$\frac{dy_2}{dt} = \frac{b_3 y_1 y_4}{b_4 + y_4} - 0.9082\, b_5\, y_2$$

Kadar pembentukan asid glukonik:
Rate of gluconic acid formation:

$$\frac{dy_3}{dt} = b_5 y_2$$

Kadar penggunaan glukosa:
Rate of glucose comsumption:

$$\frac{dy_4}{dt} = -1.011 \left(\frac{b_3 y_1 y_4}{b_4 + y_4}\right)$$

di mana *where* y_1 = kepekatan sel *concentration of cell*
y_2 = kepekatan glukonolakton *concentration of gluconolactone*
y_3 = kepekatan asid glukonik *concentration of gluconic acid*
y_4 = kepekatan glukosa *concentration of glucose*
b_1 - b_5 = sistem parameter berfungsikan suhu dan pH.
parameters of the system which are function of temperature and pH.

Pada keadaan operasi 30°C dan pH 6.6, nilai-nilai untuk kelima-lima parameter ditentukan dari data eksperimen seperti berikut:

At the operating conditions of 30°C and pH 6.6, the values of the five parameters were determined from experimental data to be:

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$b_1 = 0.949$ $b_2 = 3.439$
$b_3 = 18.72$ $b_4 = 37.51$
$b_5 = 1.167$

Pada keadaan ini, binakan profil masa untuk kesemua pembolehubah y_1 , y_2 , y_3 , y_4 untuk julat masa $0 \le t \le 3$hr.

At these conditions, develop the time profile of all variable, y_1 , y_2 , y_3 , y_4 for the period $0 \le t \le 3$hr.

Pada permulaan jangkamasa itu, nilai-nilainya adalah
At the begining of this period the values were

$y_1(0) = 0.5$ U.O.D/mL $y_2(0) = 0.0$ mg/mL

$y_3(0) = 0.0$ mg/mL $y_4(0) = 50.0$ mg/mL

Gunakan 1 jam sebagai saiz langkah anda. Selesaikan masalah tersebut dengan menunjukkan penyelesaian secara terperinci.

Take a step size of 1 hour. Solve your problem showing all details of solution.

(25 markah)

2. Satu sistem reaktor tangki teraduk berterusan (CSTR) terdiri daripada M buah tangki bersiri seperti yang ditunjukkan dalam Rajah Q2. Larutan Q (m^3/jam) disuapkan ke dalam setiap tangki. Suapan ke dalam tangki pertama mengandungi kepekatan komponen A, C_o mol /m^3. Setiap tangki diaduk dengan sempurna. Tindakbalas tak berbalik tertib pertama A $\rightarrow$ B telah berlaku di dalam setiap tangki. Kadar tindakbalas A telah diberi seperti ungkapan $-\frac{dW_n}{dt} = (kVC)_n$ mol / jam. Jika pemalar kadar tindakbalas k bagi kesemua tangki adalah sama, tunjukkan bahawa kepekatan B yang tertinggi boleh dihasilkan dengan sistem tangki ini bila $V_i = V_1 = V_2 = \ldots\ldots V_M$, dengan syarat isipadu keseluruhan $V = \sum_{n=1}^{n=m} V_n$ adalah malar.

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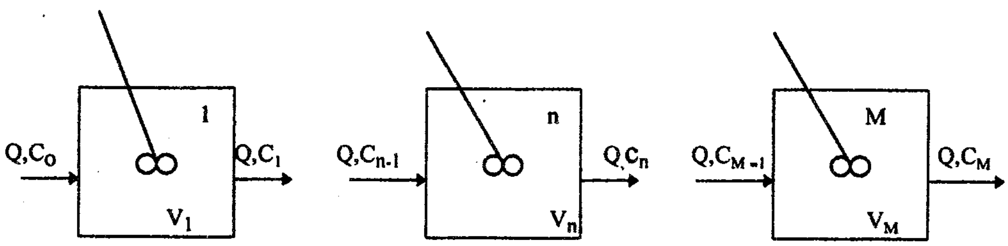
A continuous stirred-tank reactor system consists of M tanks in series, as shown in Figure Q2. $Q(m^3/h)$ of solution is fed to each tank. The feed to the first tank contains a concentration of C_o moles/m^3 of component A. Each tank is well stirred. Inside the tanks, the irreversible first-order reaction A → B takes place. The rate at which A reacts is given by the expression.

$$-\frac{dW_n}{dt} = (kVC)_n \text{ moles / hr}$$

If the reaction-rate constant k is the same for each tank, show that the highest concentration of B which may be produced by the tank system occurs when $V_i = V_1 = V_2 = \ldots\ldots V_M$, provided that the total volume $V = \sum_{n=1}^{n=m} V_n$ remains constant.



Rajah Q2: Peringkat reaktor tangki teraduk
Figure Q2: Stirred-tank reactor stages

(25 markah)

3. Asid asetik dipecahkan di dalam relau untuk menghasilkan ketene melalui tindakbalas ini.

Acetic acid is cracked in a furnace to produce the intermediate ketene via the reaction

$$CH_3COOH(g) \rightarrow CH_2CO(g) + H_2O(g)$$

Tindakbalas ini juga berlaku pada kadar yang berpatutan.

$$CH_3COOH(g) \rightarrow CH_4(g) + CO_2(g)$$

The reaction $CH_3COOH(g) \rightarrow CH_4(g) + CO_2(g)$ also occurs to an appreciable extent.

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Proses ini perlu dipecahkan pada suhu T K dengan penukaran 80% dan pecahan hasil ketene ialah 0.0722.

It is desired to carry out cracking at temperature T K with a conversion of 80% and a fractional yield of ketene of 0.0722.

Sekiranya asid asetik disuapkan ke dalam reaktor pada 300°C dan tekanan 1 Bar.

If acetic acid is fed to the reactor at 300°C and 1 Bar.

[a] Tunjukkan persamaan kepekatan untuk proses ini dan tunjukkan bagaimana kadar pemanasan yang diperlukan oleh relau boleh dikira untuk suapan 100 kg mol/jam asid.

Show the concentration equations to this process, and also show how the required furnace heating rate can be calculated for a feed of 100 kg mol/h acid.

[b] Tunjukkan rajah aliran maklumat sistem ini.

Show your information flow diagram of the system.

Data: $Cp = a + bT + CT^2 + dT^3$

	a	b	c	d
CH_2CO	4.11	2.966×10^{-2}	-1.79×10^{-3}	4.22×10^{-9}
CH_3COOH	−3.61	6.05×10^{-1}	-3.94×10^{-4}	-5.62×10^{-7}
CO_2	11.110	1.16	-7.23×10^{-3}	1.55×10^{-5}
CH_4	−5.71	1.03	-1.67×10^{-3}	1.96×10^{-5}
H_2O	18.3	0.47	-1.34×10^{-3}	1.32×10^{-6}

(25 markah)

4. Satu reaktor menukarkan sebatian organik kepada hasil P dengan bahan tambah (additive) A (pecahan mol = x_A). Bahan tambah A boleh disuntik ke dalam reaktor, dan stim boleh disuntik ke dalam lingkaran pemanas di dalam reaktor tersebut dengan tujuan pembekalan haba.

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A reactor converts an organic compound to product P by heating the material in the presence of an additive A (mole fraction = x_A). The additive can be injected into the reactor, while steam can be injected into a heating coil inside the reactor to provide heat.

Hasil P dijual pada harga RM50.00 per lb-mol. Untuk 1 lb-mol suapan, kos untuk bahan tambahan A (dalam RM per lb-mol) sebagai fungsi x_A diberi sebagai formula ini:

The product P can be sold for RM50.00 per lb-mol. For 1 lb-mol of feed, the cost of the additive (in RM per lb-mol) as a function of x_A is given by the formula:

$$0.1 + 0.5x_A + x_A^2$$

Kos wap (dalam RM) sebagai fungsi S adalah
The cost of the steam (in RM) as a function of S is

$$0.2 + 0.035S + 0.01S^2.$$

(S = paun wap/paun-mol suapan)
(S = lb steam/lb-mol feed)

Persamaan hasilan ialah $y_p = 0.1 + 0.3x_A + 0.02S + 0.001x_A S$
The yield equation is $y_p = 0.1 + 0.3x_A + 0.02S + 0.001x_A S$

y_p = paun-mol hasil/paun-mol suapan.
y_p = *lb-mol product/lb-mol feed.*

[a] Berikan fungsi keuntungan dengan x_A dan S.
Formulate the profit function in terms of x_A and S.

[b] Maksimumkan fungsi keuntungan dengan mana-mana kaedah.
Maximize the profit function using any method.

[c] Tunjukkan samada fungsi keuntungan adalah cekung atau cembong dan berikan sebabnya.
Show whether the profit function is concave or convex and why?

(25 markah)

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5. Fungsi objektif berikut telah diperolehi
The following objective function was obtained

$$f = 3x_1 + x_2 + x_3$$

yang diperlukan untuk memaksimumkan fungsi objektif berdasarkan kepada:
it is required to maximize the objective function subject to:

$$x_1 - 2x_2 + x_3 \leq 11$$

$$-4x_1 + x_2 + 2x_3 \geq 3$$

$$2x_1 - x_3 = -1$$

$$x_1, x_2, x_3 \geq 0$$

[a] Dengan menggunakan kaedah Simplex, terangkan langkah-langkah penyelesaian persamaan-persamaan itu.
Using the Simplex method explain steps of solution of these equations.

[b] Terangkan samada penyelesaian asas yang bersesuaian untuk masalah ini.
Explain whether a basic feasible solution exist for this problem.

Tunjukkan segala maklumat terperinci penyelesaian anda. <u>Anda tidak perlu mengira sebarang penyelesaian yang sesuai.</u>

Show all details of your solution. <u>You don't have to calculate the feasible solution.</u>

(25 markah)

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LAMPIRAN

Solution of non-linear Equations

1. Newton's Method:

$$f(x) = f(x_o)\ [x - x_o] + f(x_o)$$

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}$$

2. Secant Method:

$$x_{i+1} = x_i - \frac{f(x_i)(x_i - x_{i-1})}{f(x_i) - f(x_{i-1})}$$

3. Regula Falsi Method:

$$x_{i+1} = x_i - f(x_1)\frac{(x_i - x_{i-1})}{f(x_i) - f(x_i - 1)}$$

4. Illionis Method:

$$x_{i+2} = x_{i+1} - f(x_{i+1})\frac{x_{i+1} - x_{i-1}}{f(x_{i+1}) - \frac{1}{2} f(x_{i-1})}$$

5. Solution of n non-linear Equations

$$\sum_{i=1}^{n} \left.\frac{\partial f_k(x)}{\partial x_i}\right|_{x^{(j)}} d_i^{(j)} = -f_k\left[x^{(j)}\right]$$

$$k = 1,\ 2,\ \ldots\ldots n$$

$$x_i^{(j+1)} = x_i^{(j)} + d_i^{(j)}$$

i = 1,, 2, ...n
j = number of iteration.

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Solution of ODE

1. Explicit Euler method:

$$y_{i+1} = y_i + \Delta x f(x_i, y_i)$$

2. Runge-Kutta Second Order Method:

$$y_{i+1} = y_i + \frac{1}{2}(k_1 + k_2)$$

where

$$k_1 = f(x_i, y_i)$$

$$k_2 = f\left(x_i + \tfrac{1}{2} hx, y_i + k_1\right)$$

3. Implicit Mehtods:

3.1 Euler

$$y_{i+1} = y_i + \Delta x f\left(x_{i+1}, y_{i+1}\right)$$

3.2 Trapezoidal

$$y_{i+1} = y_i + \frac{\Delta x}{2}\left[f\left(x_i, y_i\right) + f\left(x_{i+1}, y_{i+1}\right)\right]$$

4. Systems of Coupled ODE'S

Runge-Kutta Second Order:

$$y_{i,j+1} = y_{i,j} + \frac{1}{2}\left(k_{1,i,j} + k_{2,i,j}\right)$$

$$k_{1,i,j} = f_i\left(x_j, y_{1,j}, y_{2,j} \ldots\ldots\ldots\ldots y_{n,j}\right)$$

$$k_{2,i,j} = f_i\left(x_j + \frac{\Delta x}{2}, y_{i,j} + \frac{\Delta x}{2} k_{1,1,j}, \ldots\ldots\ldots y_{n,j} + \frac{\Delta x}{2} k_{1,n,j}\right)$$

Table **Geometric interpretation of a quadratic function**

Case	Eigenvalue Relations	Signs α_1	Signs α_2	Types of contours	Geometric interpretation	Character of center of contours	Figure
1	$\alpha_1 = \alpha_2$	−	−	Circles	Circular hill	Maximum	4.12
2	$\alpha_1 = \alpha_2$	+	+	Circles	Circular valley	Minimum	4.12
3	$\alpha_1 > \alpha_2$	−	−	Ellipses	Elliptical hill	Maximum	4.13
4	$\alpha_1 > \alpha_2$	+	+	Ellipses	Elliptical valley	Minimum	4.13
5	$\lvert\alpha_1\rvert = \lvert\alpha_2\rvert$	+	−	Hyperbolas	Symmetrical saddle	Saddle point	4.14
6	$\lvert\alpha_1\rvert = \lvert\alpha_2\rvert$	−	+	Hyperbolas	Symmetrical saddle	Saddle point	4.14
7	$\alpha_1 > \alpha_2$	+	−	Hyperbolas	Elongated saddle	Saddle point	4.14
8	$\alpha_2 = 0$	−		Straight lines	Stationary* ridge	None	4.15
9	$\alpha_2 = 0$	+		Straight lines	Stationary* valley	None	4.15
10	$\alpha_2 = 0$	−		Parabolas	Rising ridge*†	At ∞	4.16
11	$\alpha_2 = 0$	−		Parabolas	Falling valley*†	At ∞	4.16

* These are "degenerate" surfaces.
† The condition of rising or falling must be evaluated from the linear terms in $f(\mathbf{x})$.