

UNIVERSITI SAINS MALAYSIA

Peperiksaan Semester Pertama  
Sidang Akademik 1997/98

September 1997

**EKC 370 Kaedah Pengiraan Kejuruteraan Kimia**

Masa: [3 jam]

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**ARAHAN KEPADA CALON:**

Sila pastikan soalan peperiksaan ini mengandungi **TUJUH (7)** mukasurat bercetak sebelum anda memulakan peperiksaan.

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

Jawab hanya **EMPAT (4)** soalan sahaja.

**SATU (1)** soalan **MESTI** dijawab dalam Bahasa Malaysia.

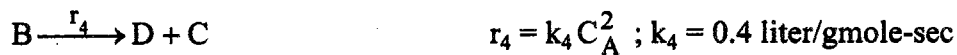
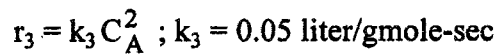
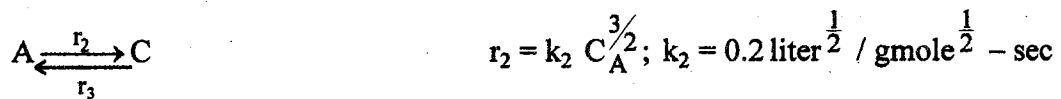
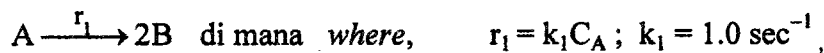
Peperiksaan ini dijalankan secara 'Open Book'.

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1. (Kaedah Newton-Raphson *Newton-Raphson Method*)

Satu reaktor tangki teraduk selanjur (CSTR) yang berisipadu  $V = 100$  liter mempunyai tindakbalas seperti berikut (fasa cecair):

*Consider a continuously stirred tank reactor (CSTR) of volume  $V = 100$  liters in which the following reactions take place in liquid phase:*



Volumetric suapan ke dalam reaktor ialah  $Q = 50$  liter/sec pada kepekatan  $C_{A_0} = 1.0$  gmole/liter bagi komponen A.

*The volumetric feed to the reactor is  $Q = 50$  liters/sec at a concentration of  $C_{A_0} = 1.0$  gmole/liter of component A.*

Oleh kerana reaktor (CSTR) itu direka untuk beroperasi pada keadaan mantap dan sistem itu dianggap berada pada keadaan isotermik, keseimbangan mol yang mendefinisikan prestasinya adalah seperti berikut:

*Since a CSTR is designed to operate at steady state and this system is assumed to be operated under isothermal conditions, the following steady-state mole balances define the performance of the system:*

	Out	=	In	+	Janaan Generation	-	Penggunaan Consumption
Komponen A: (Component A):	$C_A Q$	=	$C_{A0} Q$	+	$V(r_3)$	-	$V(r_1 + r_2)$
Komponen B: (Component B):	$C_B Q$	=	0	+	$V(2r_1)$	-	$V(r_4)$
Komponen C: (Component C):	$C_C Q$	=	0	+	$V(r_2 + r_4)$	-	$V(r_3)$
Komponen D: (Component D):	$C_D Q$	=	0	+	$V(r_4)$	-	0

Dengan menggantikan ungkapan kadaran, anda akan mendapat empat persamaan algebra tak linear dengan empat anu ( $C_A$ ,  $C_B$ ,  $C_C$  dan  $C_D$ ). Selesaikan persamaan-persamaan tersebut menggunakan kaedah Newton. Anggapkan nilai berikut sebagai andaian permulaan:

$$C_A^{(0)} = C_B^{(0)} = C_C^{(0)} = C_D^{(0)} = 0.30 \text{ gmole/liter}$$

*Substituting the rate expressions, you will have four nonlinear algebraic equations with four unknowns ( $C_A$ ,  $C_B$ ,  $C_C$  and  $C_D$ ). Solve these equations using Newton's method. Assume the following values as your initial guess:*

$$C_A^{(0)} = C_B^{(0)} = C_C^{(0)} = C_D^{(0)} = 0.30 \text{ gmole/liter.}$$

(25 markah)

2. (Perumusan Fizikal *Physical Formulation*)

Sebiji bebola pil berasaskan membran berjejari  $R$  dimasukkan ke dalam badan manusia bertujuan untuk meresapkan dadah A secara terkawal ke dalam bendalir psikologi manusia. (Cabang baru dalam kejuruteraan kimia ini dinamakan "Pelepasan Terkawal"). Semasa dadah itu meresap ke dalam badan, ia melalui tindakbalas tak berbalik, tertib pertama.

*A spherical membrane-based pill of radius  $R$  is inserted into a human body to provide a controlled release of a drug A into the physiological fluid of the human body (this new branch of chemical engineering is called "Controlled Release"). As the drug diffuses through the pill into the body, it undergoes an irreversible, first-order chemical reaction.*

- [a] Tuliskan keseimbangan jisim pada keadaan mantap untuk dadah A di dalam badan. Terbitkan satu persamaan ODE untuk kepekatan dadah di sekeliling pil tersebut.

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*Write down a steady-state mass balance for the drug A in the body, and derive an ODE for the concentration of drug around the pill.*

(15 markah)

- [b] Tuliskan keadaan sempadannya.  
*Write down the boundary conditions.*

(5 markah)

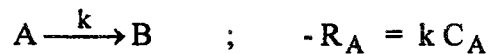
- [c] Tuliskan penyelesaian untuk sistem di atas.  
*Write down the solution to the above system.*

(5 markah)

3. (ODE: Penyelesaian Berangka ODE: Numerical Solution)

Pertimbangkan resapan dan tindakbalas di dalam liang silinder sepanjang L di mana komponen A bertindakbalas di dinding silinder tersebut berdasarkan:

*Consider diffusion and reaction in a cylindrical pore of length L where component A reacts at the walls of the cylinder according to*



Di dalam sistem ini, A meresap melalui liang tersebut sementara itu bertindakbalas pada permukaan dinding liangnya. Pada saluran kemasukan diliang ( $x = 0$ ), kepekatan A ialah  $C_{A0}$ . Andaikan pada penghujung akhir liang itu ditutup. Apabila dilakukan keseimbangan mol pada keadaan mantap untuk isipadu kebezaan sistem itu, keputusannya adalah seperti berikut (ODE):

*In this system, A diffuses into the pore and, meanwhile, reacts at the surface of the pore wall. At the inlet of the pore (i.e.,  $x = 0$ ), the concentration of A is  $C_{A0}$ . The end of the pore is assumed to be closed off. Performing a steady-state mole balance for a differential volume of the system results in the following ODE:*

$$D_A \frac{d^2 C_A}{dx^2} = k C_A ; \text{ di mana } C_A \text{ ialah purata luas keratan kepekatan A .}$$

$$D_A \frac{d^2 C_A}{dx^2} = k C_A ; \text{ where } C_A \text{ is the cross-sectional average concentration of A .}$$

Keadaan sempadan untuk masalah ini ialah: 
$$\begin{cases} C_A = C_{A0} & @ x = 0 \\ dC_A / dx = 0 & @ x = L \end{cases}$$

The boundary conditions for this problem are: 
$$\begin{cases} C_A = C_{A0} & @ x = 0 \\ dC_A / dx = 0 & @ x = L \end{cases}$$

Dengan kaedah perbezaan terhingga, selesaikan BVP, dengan menggunakan nilai-nilai di bawah:

*Use finite-difference method to solve this BVP, using the following values:*

$$k = 0.01 \text{ sec}^{-1}; C_{A0} = 1.0 \text{ gmole/liter}; D_A = 1.0 \times 10^{-3} \text{ cm}^2/\text{sec}; L = 1.0 \text{ cm}$$

Gunakan:  $\Delta x = 0.2$  sebagai langkah jejaring dan "Thomas Algorithm" untuk menyelesaikan persamaan matrik tridiagonal.

*Use:  $\Delta x = 0.2$  as your mesh step, and use "Thomas Algorithm" to solve the tridiagonal matrix equation.*

(25 markah)

4. (PDE: Penyelesaian Berangka PDE: Numerical Solution)  
Gunakan teknik berangka "Successive Over-Relaxation (S.O.R.)" untuk menerbitkan sistem persamaan-persamaan terasing berikut:

*Use the numerical technique of Successive Over-Relaxation (S.O.R.) to derive the discretized forms for the following parabolic system equations:*

$$\text{PDE: } \frac{\partial C_A}{\partial t} = \left( \frac{\partial^2 C_A}{\partial r^2} + \frac{1}{r} \frac{\partial C_A}{\partial r} \right) - \frac{k}{D_A} C_A \quad (r > R, t > 0)$$

$$\text{BC' s: } \begin{cases} C = C_{A0} & @ r = R \\ \partial C_A / \partial r = 0 & @ r \rightarrow \infty \end{cases} \quad (t > 0)$$

$$\text{IC: } C_A = 0 \quad @ t = 0 \quad (r \geq R)$$

Data:

$$R = 1.0 \text{ cm}$$

$$k = 0.01 \text{ sec}^{-1}$$

$$D_A = 1 \times 10^{-5} \text{ cm}^2 / \text{sec}$$

$$C_{A0} = 0.2 \text{ gmole / liter}$$

Gunakan *use*:  $h = \Delta r = 0.25$ ,  $k = \Delta t = 0.5$ ,  $\rho = k/h^2$ ,  $\omega = 1.20$

Jangan selesaikan persamaan-persamaan berikut.

*Do not solve the discretized equations.*

(25 markah)

5. (PDE: Penyelesaian Analitikal *PDE: Analytical Solution*)

Selesaikan sistem berikut secara analitikal:

*Solve the following system analytically:*

$$\begin{cases} \text{PDE: } u_t = u_{xx} + \sin(\pi x) & (0 < x < 1.0; t > 0) \\ \text{BC' s: } u(0, t) = 1; u(1, t) = 0 & (t > 0) \\ \text{IC: } u(x, 0) = \exp(-x) & (0 \leq x \leq 1.0) \end{cases}$$

[a] Mula-mula, jadikan keadaan sempadan (BC) homogen.

*First make the BC's homogeneous.*

(15 markah)

[b] Kemudian, selesaikan sistem ini dengan menggunakan kaedah "Pemisahan Pembolehubah".

*Then solve the system by the "Separation of Variables" method.*

(5 markah)

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- [c] Lukiskan rajah berskema untuk kelakuan sistem tersebut:  $u(x,t)$  berlawan  $x$  dan  $t$ .

*Draw a schematic diagram of the system behaviour:  $u(x,t)$  versus  $x$  and  $t$ .*

(5 markah)

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