UNIVERSITI SAINS MALAYSIA

Second Semester Examination
2010/2011 Academic Session

April/May 2011

EKC 245 – Mathematical Methods For Chemical Engineering
[Kaedah Matematik Kejuruteraan Kimia]

Duration : 3 hours
[Masa : 3 jam]

Please ensure that this examination paper contains SIX printed pages and THREE printed page of Appendix before you begin the examination.

[Sila pastikan bahawa kertas peperiksaan ini mengandungi ENAM muka surat yang bercetak dan TIGA muka surat Lampiran 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].

1. The concentration of biochemical oxygen demand (BOD), *m*, in a wastewater treatment tank decreases according to

Kepekatan keperluan oksigen biokimia (BOD), m, *di dalam tangki rawatan air sisa berkurang berdasarkan*

$$m = 75e^{-1.5t} + 20e^{-0.075t}$$

Determined the time, t required for the BOD concentration to be reduced to 15 using Newton-Raphson method with initial guess of t = 6 and a stopping criterion of 0.5%. Verify your result.

Tentukan masa, t yang diperlukan bagi mengurangkan kepekatan BOD kepada 15 dengan menggunakan kaedah Newton-Raphson, anggaran awal t = 6 dan kriteria berhenti 0.5%. Buktikan keputusan anda.

[25 marks/markah]

2. Figure Q.2. shows three reactors linked by pipes. As indicated, the rate of transfer of chemicals through each pipe is equal to a flowrate (Q, with units of cubic meters per second) multiplied by the concentration of the reactor from which the flow originates (c, with units of milligrams per cubic meter). If the system is at a steady state, the transfer into each reactor will balance the transfer out. The flowrates are given as $Q_{13} = 20$, $Q_{12} = 45$, $Q_{21} = 15$, $Q_{23} = 30$ and $Q_{33} = 60$. Develop mass-balance equations for the reactors and indentify their concentrations using

Rajah S.2. menunjukkan tiga reaktor dihubungkan dengan paip. Seperti tertera, kadar pemindahan bahan kimia melalui setiap paip bersamaan dengan kadar alir (Q, dengan unit meter padu per saat) didarab dengan kepekatan reaktor daripada aliran asal tersebut (c, dengan unit milligram per meter padu). Jika sistem tersebut dalam keadaan mantap, pemindahan masuk ke setiap reaktor seimbang dengan pemindahan keluar. Kadar aliran diberi sebagai $Q_{13} = 20$, $Q_{12} = 45$, $Q_{21} = 15$, $Q_{23} = 30$ *dan* $Q_{33} = 60$. *Terbitkan persamaan keseimbangan jisim untuk semua reaktor dan tentukan kepekatan masing-masing menggunakan*

[a] Gauss elimination method
Kaedah penyisihan Gauss

[b] Gauss-Seidel method
Kaedah Gauss-Siedel

[25 marks/markah]

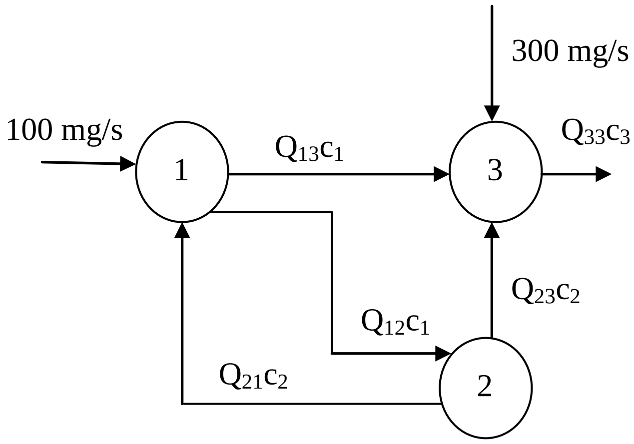

Figure Q.2.
Rajah S.2.

3. [a] A temperature function across a board is
Fungsi suhu merentasi satu papan ialah

$$f(x,y) = 5x^2 - xy + y^2 + 3y$$

[i] Find the maximum temperature based on analytical solution.
Carikan suhu maksima berdasarkan penyelesaian analitikal.

[6 marks/markah]

[ii] Perform two iteration of steepest ascent method on the function starting at point (1,1).
Lakukan dua lelaran kaedah naik tercuram pada fungsi tersebut bermula dari titik (1,1).

[8 marks/markah]

[iii] List out the advantages and disadvantages of steepest ascent/descend method.
Senaraikan kebaikan dan keburukan kaedah naik/turun tercuram.

[4 marks/markah]

[b] Reactant *A* is being converted into product *X* in a system. The rate of reaction for each species is given as follows:

Bahan tindak balas A ditukar kepada produk X dalam suatu sistem. Kadar tindak balas bagi setiap spesis adalah diberi seperti di bawah:

$$\frac{dC_A}{dt} = -k_1 C_A{}^2 + k_2 C_X$$

$$\frac{dC_X}{dt} = \frac{k_1 C_A{}^2}{1 + K C_X}$$

where C_i = concentration of species i; t = time in s and rate constants k_1 = 0.514 (mol/ dm^3)$^{-1}$s^{-1}; k_2 = 0.238 s^{-1} ; K = 0.752 (mol/ dm^3)$^{-1}$. Find the concentration of *A*, and *X* after 1 s. The initial feed to the reactor is pure A with concentration 2 mol/dm^3.

di mana C_i = kepekatan spesis i; t = masa dalam saat dan pemalar kadar k_1 = 0.514 (mol/ dm^3) $^{-1}$s^{-1}; k_2 = 0.238 s^{-1} ; K = 0.752 (mol/ dm^3)$^{-1}$. Carikan kepekatan A dan X selepas 1 saat. Suapan awal ke reaktor ialah A tulen dengan kepekatan 2 mol/dm^3.

[7 marks/markah]

4. [a] [i] A heated plate is subjected to two boundary temperatures held at constant value (in degree Celsius) at certain positions and two boundaries being insulated as shown in Figure Q.4.[a]. Use Liebmann's method to solve for the temperature at the nodes in the grid (calculate the temperature at 6 points) of the heated plate to compute the steady state distribution of temperature. Employ overrelaxation with a value of 1.5 for the weighting factor and iterate 1 time. Start from the point i =1, j = 0 with the assumption that all the unknown points are zeros.

Sebuah plat panas dengan dua suhu sempadan yang dikekal (darjah Celsius) pada suhu tetap di titik-titik tertentu dan dua sempadan ditebat adalah ditunjukkan dalam Rajah S.4.[a]. Gunakan kaedah Liebmann untuk menyelesaikan suhu di titik-titik grid (kirakan suhu bagi 6 titik) pada plat panas untuk mencari taburan suhu pada keadaan mantap. Gunakan santaian dengan nilai 1.5 bagi faktor pemberat dan lelar 1 kali. Mula dari titik i =1, j = 0 dengan anggapan bahawa semua titik anu adalah sifar.

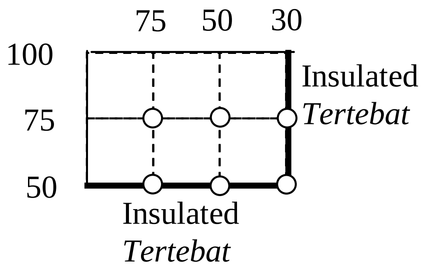

Figure Q.4.[a].
Rajah S.4.[a].

[10 marks/markah]

[ii] Given the temperature (in degree Celsius) distribution of a heated plate at steady state is given as shown in Figure Q.4.[b]. Calculate the fluxes for the two nodes in the grid of the plate.

Taburan suhu (dalam darjah Celsius) bagi sebuah plat panas pada keadaan mantap adalah seperti dalam Rajah S.4.[b]. Hitungkan fluks bagi dua titik pada plat panas tersebut.

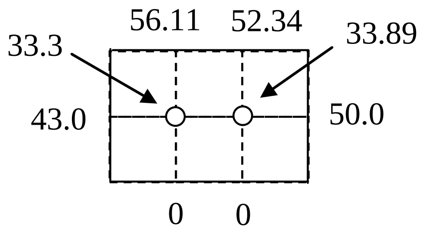

Figure Q.4.[b].
Rajah S.4.[b].

Assume that the plate is 20 cm x 30 cm and is made out of aluminum.
Anggapkan plat tersebut adalah 20 sm x *30 sm dan diperbuat daripada aluminium.*

[k'= 0.49 cal/s.cm.^{o}C]

Hint: Fourier's law of heat conduction:
Petunjuk: Hukum Fourier bagi konduksi haba:

$q_i = -k'\frac{\partial T}{\partial i}$ where q_i = heat flux in the direction of the i dimension [cal/cm^2.s]

$q_i = -k'\frac{\partial T}{\partial i}$ *di mana q_i = fluks haba pada arah dimensi i [cal/sm^2.s]*

[5 marks/markah]

[b] A 4 cm long thin rod is insulated at all point except at its ends. At time t = 0, the temperature of the whole rod is 30^{o}C and the boundary conditions are fixed for all times at T(0) = 120^{o}C and T(10) = 45^{o}C. Given Δx = 1 cm, Δt = 1 s and k = 0.944 cm^2/s. Calculate the temperature distribution at t = 1s using the simple implicit method. The Laplacian difference equations for the system is given as

Satu rod halus yang panjangnya 4 sm ditebat pada semua titik kecuali pada kedua-dua hujungnya. Pada masa t = 0, suhu seluruh rod tersebut ialah 30^{o}C dan keadaan sempadan dikekal pada T(0) = 120^{o}C dan T(10) = 45^{o}C. Diberi Δx = 1 sm, Δt = 1 s dan k = 0.944sm^2/s. Kirakan taburan suhu pada t = 1s menggunakan kaedah implisit mudah. Persamaan Laplace bagi sistem tersebut diberi sebagai

$$-\lambda T_{i-1}^{l+1} + (1+2\lambda)T_i^{l+1} - \lambda T_{i+1}^{l+1} = T_i^l \quad \text{where } \lambda = k\,\Delta t/(\Delta x)^2$$

[10 marks/markah]

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Appendix

Matrix of Polynomial Regression

$$\begin{bmatrix} n & \sum x_i & \sum x_i^2 \\ \sum x_i & \sum x_i^2 & \sum x_i^3 \\ \sum x_i^2 & \sum x_i^3 & \sum x_i^4 \end{bmatrix} \begin{Bmatrix} a_o \\ a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} \sum y_i \\ \sum x_i y_i \\ \sum x_i^2 y_i \end{Bmatrix}$$

Matrix of Multiple Linear Regression

$$\begin{bmatrix} n & \sum x_{1i} & x_{2i} \\ \sum x_{1i} & \sum x_{1i}^2 & \sum x_{1i} x_{2i} \\ \sum x_{2i} & \sum x_{1i} x_{2i} & \sum x_{2i}^2 \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{Bmatrix} \sum y_i \\ \sum x_{1i} y_i \\ \sum x_{2i} y_i \end{Bmatrix}$$

Differentiation Formulas

Forward finite-divided-difference

First derivative

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

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} \qquad O(h^2)$$

Second derivative

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} \qquad O(h)$$

$$f''(x_i) = \frac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2} \qquad O(h^2)$$

Backward finite-divided-difference

First derivative

$$f'(x_i) = \frac{f(x_1) - f(x_{i-1})}{h} \qquad O(h)$$

$$f'(x_i) = \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h} \qquad O(h^2)$$

Second derivative

$$f''(x_i) = \frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2} \qquad O(h)$$

$$f''(x_i) = \frac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3})}{h^2} \qquad O(h^2)$$

…2/-

Centred finite-divided-difference

First derivative
$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} \qquad O(h^2)$$
$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h} \qquad O(h^4)$$

Second derivative
$$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2} \qquad O(h^2)$$
$$f''(x_i) = \frac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2} \qquad O(h^4)$$

Derivatives of unequally spaced data

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

Integration Formulas

Trapezoidal Rule

$$I = (a - b)\frac{f(a) + f(b)}{2}$$
$$I = (b - a)\frac{f(x_o) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)}{2n}$$

Simpson's 1/3 Rule

$$I \cong (b - a)\frac{f(x_o) + 4f(x_1) + f(x_2)}{6}$$

$$I \cong (b - a)\frac{f(x_o) + 4\sum_{i=1,3,5}^{n-1} f(x_i) + 2\sum_{j=2,4,6}^{n-2} f(x_j) + f(x_n)}{3n}$$

Useful Formula

ODE solver

Euler's method

$y_{i+1} = y_i + y_i'h$

4th order Runge-Kutta

$y_{i+1} = y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h$

where $k_1 = f(x, y)$

$k_2 = f(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h)$

$k_3 = f(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_2 h)$

$k_4 = f(x_i + h, y_i + k_3 h)$

Finite difference methods

Laplacian difference equations

$T_{i+1,j} + T_{i-1,j} + T_{i,j+1} + T_{i,j-1} - 4\,T_{i,j} = 0$

Explicit method:

$$\frac{\partial T}{\partial t} \cong \frac{T_i^{l+1} - T_i^l}{\Delta t}; \qquad \frac{\partial^2 T}{\partial x^2} = \frac{T_{i+1}^l - 2T_i^l + T_{i-1}^l}{\Delta x^2}$$

Simple implicit method:

$$\frac{\partial T}{\partial t} \cong \frac{T_i^{l+1} - T_i^l}{\Delta t}; \qquad \frac{\partial^2 T}{\partial x^2} \cong \frac{T_{i+1}^{l+1} - 2T_i^{l+1} + T_{i-1}^{l+1}}{(\Delta x)^2}$$

The Crank Nicolson Method

$$\frac{\partial T}{\partial t} \cong \frac{T_i^{l+1} - T_i^l}{\Delta t}; \qquad \frac{\partial^2 T}{\partial x^2} \cong \frac{1}{2}\left[\frac{T_{i+1}^l - 2T_i^l + T_{i-1}^l}{(\Delta x)^2} + \frac{T_{i+1}^{l+1} - 2T_i^{l+1} + T_{i-1}^{l+1}}{(\Delta x)^2}\right]$$

Overrelaxation

$$T_{i,j}^{new} = \lambda T_{i,j}^{new} + (1-\lambda) T_{i,j}^{old}$$