Name : .....

Roll No. : .....

Invigilator's Signature : .....

CS/B.Tech (CHE-OLD)/SEM-6/CHE-604/2013

2013

NUMERICAL METHODS IN CHEMICAL ENGINEERING

Time Allotted : 3 Hours *Full Marks* : 70

The figures in the margin indicate full marks.
Candidates are required to give their answers in their own words as far as practicable.

GROUP – A
(Multiple Choice Type Questions)

1. Choose the correct alternatives for any *ten* of the following : $10 \times 1 = 10$

i) For an equation like $x^2 = 0$, a root exists at $x = 0$. The bisection method cannot be adopted to solve this equation in spite of the root existing at $x = 0$ becuase the function $f(x) = x^2$

a) is a polynomial

b) has repeated roots at $x = 0$

c) is always non-negative

d) slope is zero at $x = 0$.

ii) The secant method formula for finding the square root of a real number R from the equation $x^2 - R = 0$ is

a) $\dfrac{x_i\, x_{i-1} + R}{x_i + x_{i-1}}$ b) $\dfrac{x_i\, x_{i-1}}{x_i + x_{i-1}}$

c) $\dfrac{1}{2}\left(x_i + \dfrac{R}{x_i}\right)$ d) $\dfrac{2x_i^{\,2} + x_i\, x_{i-1} - R}{x_i + x_{i-1}}$.

iii) In final value problem, the values of the dependent variable and/or their derivatives are all known

a) at the final value of the independent variable

b) at the initial and final value of the independent variable

c) at any value of the independent variable

d) at more than one point of the independent variable.

iv) If for a real continuous function $f(x), f(a)f(b)<0$, then in the range of $[a,b]$ for $f(x)=0,$ there is (are)

a) one root

b) undeterminable number of roots

c) no root

d) at least one root.

v) Modified Euler's Method is

a) implicit method b) explicit method

c) both of these d) none of these.

vi) Pivoting is very much essential because

a) Determinant of the coefficient matrix should be greater than zero

b) Pivot element should not have very large value compared to the elements of the matrix

c) It reduces the possibility of division by zero

d) Chance of convergence is higher.

vii) Least square method is used to derive

a) A curve that maximize the discrepancy between the data points and the curve

b) A curve that minimize the discrepancy between the data points and the curve

c) A straight line that maximize the discrepancy between the data points and the curve

d) A straight line that minimize the discrepancy between the data points and the curve.

viii) Simpson's 1/3 formula always requires

a) even number of ordinates

b) odd number of ordinates

c) even or odd number of ordinates

d) none of these.

ix) Secant methods are used to calculate the roots of the functions whose

a) derivatives are zero

b) derivatives are very large

c) derivatives are very small

d) derivatives may be extremely difficult or inconvenient to evaluate.

x) In trapezoidal Rule, the order of h in the total error is

a) 3 b) 4

c) 2 d) none of these.

xi) When Gauss elimination method is used to solve $AX = B$, A is transformed to a

a) unit matrix

b) lower triangular matrix

c) diagonally dominant matrix

d) upper triangular matrix.

xii) In successive over relaxation method the value of relaxation parameter varies

a) between 1 and 2 b) between 0 and 1

c) between –1 and 1 d) between –1 and 0.

GROUP – B

(Short Answer Type Questions)

Answer any *three* of the following. $3 \times 5 = 15$

2. a) Prove that the rate of convergence of Newton - Raphson method is quadratic.

b) What does speed of convergence signify ? 4 + 1

3. Find the bubble point of a binary system liquid mixture (40 mole % A and 60 mole % B) at 760·0 mm Hg.

In $P^{sat}(A) = \dfrac{-3998 \cdot 352}{T} + 17 \cdot 9$

In $P^{sat}(B) = \dfrac{-5764 \cdot 721}{T} + 21 \cdot 764$

P in mm of Hg. and T in K. Using secant method assume the liquid mix is ideal and $T_{10} = 95 \cdot 0^{\circ}\text{C}$ and $T_{20} = 90 \cdot 0\,^{\circ}\text{C}$. 5

4. a) Explain why Gauss - Seidel iterative method is not suitable for solving the following system of equations.

$x + y + z = 3$

$x + y - z = 1$

$x - y + z = 1$

b) Illustrate the concept of truncation error. 4 + 1

5. a) Let X_T and X_A denote respectively the true and approximate values of a number. Define the absolute error, relative error and percentage error in X_A.

b) Explain when the relative error is better indicator of the accuracy of a computation than the absolute error. 3 + 2

6. a) Give an example of boundary value problem.

b) Solve $\frac{dy}{dx} = x \cdot y$ for $x = 1$ taking $h = 0{\cdot}5$

initial condition : $y(0) = 1$ 1 + 4

GROUP – C

(Long Answer Type Questions)

Answer any *three* of the following. $3 \times 15 = 45$

7. a) For CH_3Cl (Methyl Chloride), following physical properties are given :

Vapour pressure (60°C) = 13·76 bar, $P_c = 66 \cdot 8$ bar, $T_c = 416 \cdot 3$ K, W = 0·153. It obeys the RK equation.

$$P = \frac{RT}{V-b} - \frac{a}{T^{1/2} V (V+b)}$$

where

$$a = \frac{0 \cdot 42748 R^2 - T_C^{2 \cdot 5}}{P_C} \text{ and } b = \frac{0 \cdot 08664 RT_C}{P_C}$$

Find the molar volume of saturated liquid using Newton-Raphson method with initial guess $V^0 = b$. How can you get the molar volume of saturated vapour ? What is the basis of obtaining the initial guess for any iterative method to be applicable for practical problem ?

b) Deduce Secant formula from Newton-Raphson formula. What is the advantage of Secant Method ? 12 + 3

8. a) Describe TDMA based on following linear system :

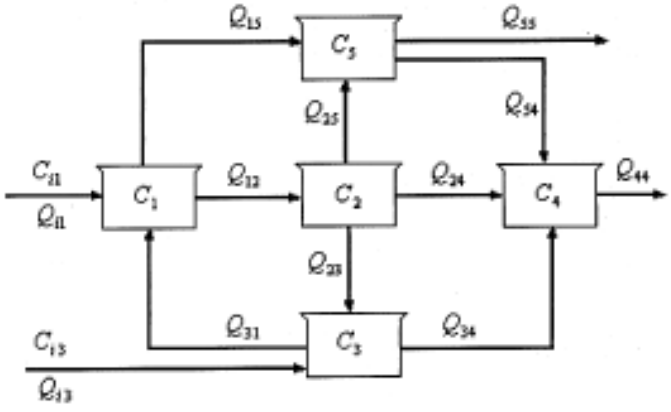
A11* × 1 + A12* × 2 = D1

A21* × 1 + A22* × 2 + A23* × 3 = D2

A31* × 1 + A32* × 2 + A33* × 3 = D4

What are the practical applications of TDMA ?

b) The system shown below is at steady state. Compute the concentration of five tanks using Gauss-Seidel iterative method with relaxation factor 1·5, if the flows are given by



$Q_{i1} = 5$; $C_{i1} = 10$

$Q_{12} = 3$; $Q_{15} = 3$

$Q_{24} = 1$; $Q_{25} = 1$; $Q_{23} = 1$

$Q_{i3} = 8$; $C_{i3} = 20$

$Q_{31} = 1$; $Q_{34} = 7$

$Q_{44} = 11$

$Q_{55} = 3$; $Q_{54} = 3$

Make minimum 3 iteration.

The system is well mixed and the concentration is uniform throughout the tank. All C_i is given in mg/ m^3 and the flow rates are given in m^3 /min. 8 + 7

9. a) Using Runga-Kutta method of order four with h = 1 find y (1), given $y' = y - x^2$, $y(0)$ = 1·5.

b) You perform the experiments and determine the following values of heat capacity C at various temperatures T for a gas :

T	–50	–30	0	60	90	110
C	1270	1280	1350	1480	1580	1700

Determine a linear and quadractic model to predict C as as a function of T. Calculate $\sum R_i^2$ 6 + 9

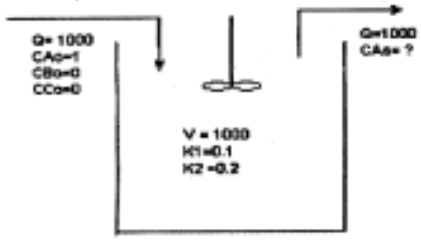
10. a) A series occurring in a CSTR of volume 1000lt

$$A \xrightarrow{K_1} B \xrightarrow{K_2} C$$

$K_1 = 0 \cdot 1 \text{ hr}^{-1}$, $K_2 = 0 \cdot 2 \text{ hr}^{-1}$

Inlet concentration by A is 1 mol/lt, $C_{BO} = 0$, $C_{CO} = 0$

Find the concentration at time 12, 15, 20 minutes also find the steady state concentration.



b) Solve $f(x) = x^3 - 5x^2 + 7x - 3 = 0$ by Newton Raphson Method, It is observed that a good initial guess like $x^{(0)} = 0$ requires a large number of iterations to find one root at $x = 1$.

Justify the above observation and suggest some modification to reduce the number of iterations. 9 + 6

11. a) Consider a steel plate of size of 15 × 15 sq. cm. If two of the sides are held at 200°C and other two sides are held at 0°C. What are the steady state temperature at interior point assuming grid size 5 × 5 sq. cm. (solve the set of equation by Gauss-elimination method)

b) Apply Crank-Nicholson Method to solve the unsteady-state conduction problem :

Where : IC : $T(x, 0) = 100\ (1 - x^2)$

BC : T (0, T) = 100·0

T (1, t) = 0·0

Assuming $M = (\Delta x)^2 / \Delta t / \alpha = 2 \cdot 5$ and $\alpha = 1 \cdot 0$ and the rectangular heat slab consists of four equal slices, compute the temperature profile with length. 5 + 10