NUMERICAL METHODS IN CHEMICAL ENGINEERING
(CHEN 3104)

Time Allotted : 2½ hrs **Full Marks : 60**

Figures out of the right margin indicate full marks.

Candidates are required to answer Group A and any 4 (four) from Group B to E, taking one from each group.

Candidates are required to give answer in their own words as far as practicable.

Group – A

1. Answer any twelve: **12 × 1 = 12**

Choose the correct alternative for the following

(i) Newton-Raphson method to solve nonlinear equation is a _____ method.
(a) Open (b) Bracket (c) Graphical (d) Random

(ii) Gauss Elimination method yields _____ matrix.
(a) Identity (b) Lower triangular
(c) Upper triangular (d) Diagonal

(iii) The local truncation error for the Euler's method is of the order of
(a) h^2 (b) h (c) h^3 (d) h^4

(iv) The local truncation error for a 4th order method for solving ODEs is of the order of
(a) h^3 (b) h^4
(c) h^5 (d) h^2

(v) For an ODE where the dependent variable changes abruptly with the independent variable, which of the following solution methods will be more suitable?
(a) Heun's method (b) 4th order R K method
(c) Ralston's method (d) Adaptive R K method

(vi) During quadratic spline with four data points number of unknowns will be equal to _____.
(a) 2n (b) 3n (c) 4n (d) 5n

(vii) The order of truncation error during finding a value for second order differentiation using forward difference scheme is _____
(a) square of the interval between independent variables
(b) cube of the interval between independent variables
(c) the interval between independent variables
(d) either (a) or (c)

(viii) Condition number equal to 1 manifests _____.
(a) the reflection of error in the independent variable (b) the reflection of error in the function
(c) the attenuation of error (d) the magnification of error

(ix) Hessian of a function 'f' is given as _____.

(a) $|H| = \frac{\partial^2 f}{\partial x^2}\frac{\partial^2 f}{\partial y^2} - \left(\frac{\partial^2 f}{\partial x \partial y}\right)^2$ (b) $|H| = \frac{\partial^2 f}{\partial x^2}\frac{\partial^2 f}{\partial y^2} + \left(\frac{\partial^2 f}{\partial x \partial y}\right)^2$

(c) $|H| = \left(\frac{\partial^2 f}{\partial x \partial y}\right)^2 - \frac{\partial^2 f}{\partial x^2}\frac{\partial^2 f}{\partial y^2}$ (d) $|H| = \left(\frac{\partial^2 f}{\partial x^2}\frac{\partial^2 f}{\partial y^2}\right)^2 - \left(\frac{\partial^2 f}{\partial x \partial y}\right)^2$

(x) Accuracy refers to how closely _____
(a) individual computed ormeasured values agree with each other
(b) individual computed ormeasured values agree with true value
(c) approximate values agree with each other
(d) approximate values agree with true value

Fill in the blanks with the correct word

(xi) The value for reverse golden ratio is equal to _____.

(xii) The number of unknown constants in quadratic spline for 'n+1' number of data points is _____.

(xiii) The discrepancy introduced by the omission ofsignificant figures is called_____ errors.

(xiv) Occurrences of both local and global optima in an optimization are called _____.

(xv) Expression of a floating with fractional part point number is called _____.

Group - B

2. (a) What is the difference between remainder and truncation error? Explain with an example. *[(CO1)(Understand/LOCQ)]*

(b) Show the binary conversion of 0.125after normalization with exponent '-2'. *[(CO1)(Apply/IOCQ)]*

(c) The following data defines the sea-level concentration of dissolved oxygen for fresh water as a function of temperature:

T^oC	0	8	16	24	32	40
C_0, mg/L	14.621	11.843	9.870	8.418	7.305	6.413

Find out the concentration at 27^oC using Newton's backward difference interpolation scheme. *[(CO2)(Analyse/HOCQ)]*

3 + 3 + 6 = 12

3. (a) A chemical reaction shows the variation of reactant concentration with time according to an exponential equation given below. The steady state of the reaction is obtained by evaluating the roots of the equation using Secant method. Show two iterations with initial guess for t=12 mins and 16 mins.

$$\frac{dC}{dt}=\frac{667.38}{t}\left[1-\exp\left(-\frac{t}{681}\right)\right]$$

[(CO3)(Analyse/IOCQ)]

(b) In between false position method and bisection method, which method will provide less number of iterations to evaluate a root of a nonlinear equation? *[(CO3)(Remember/LOCQ)]*

(c) Show that the first order polynomial can be written as $f_1(x)=f(x_0)+(x-x_0)f[x_0,x_1]$. *[(CO2)(Apply/IOCQ)]*

8 + 2 + 2 = 12

Group - C

4. (a) The below figure shows separators with flow rates 10 unit, x_1 unit, x_2 unit and x_3 unit. The mass fraction is given as 'w' for individual streams. Find out the values of x_i, i=1,2,3 using Gauss Jordon elimination.

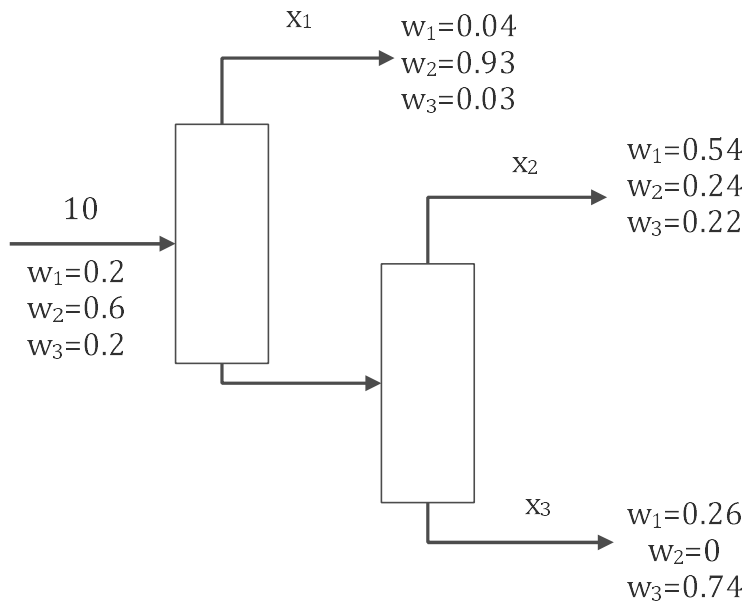

Fig. 1

[(CO2)(Analyse/HOCQ)]

(b) Write down the algorithm for Gauss Siedel method? *[(CO2)(Remember/LOCQ)]*

(c) In between Gauss Siedel and Jacobi iteration, which one shows less number of iterations to provide the roots and why? *[(CO2)(Apply/IOCQ)]*

8 + 2 + 2 = 12

5. (a) Show that the truncation error evolved for an integration using Trapezoidal method with lower and upper limit 'a' and 'b' respectively is given by $-\frac{(b-a)^3}{12}f''(\xi), a<\xi<b$

[(CO1)(Apply/IOCQ)]

(b) In an attempt to understand the mechanism of the depolarization process in a fuel cell, an electro-kinetic model for mixed oxygen-methanol current on platinum was developed in the laboratory. A very simplified model of the reaction developed suggests a functional relation in an integral form. To find the time required for 50% of the oxygen to be consumed is given by), the time, T is given by $T=-\int_{1.22\times10^{-6}}^{0.61\times10^{-6}}\left(\frac{6.73c+4.3025\times10^{-7}}{2.316\times10^{-11}c}\right)dc$

'c' is the oxygen concentration. Use single segment Trapezoidal rule to find the time required for 50% of the oxygen to be consumed, when initial oxygen level is 1.22 µg/l. *[(CO1) (Evaluate/HOCQ)]*

(c) "Simpon's $1/3^{rd}$ method will provide less error compared to Simpson's $3/8^{th}$ method" – Justify the appropriateness of the statement. *[(CO1)(Evaluate/HOCQ)]*

6 + 4 + 2 = 12

Group - D

6. (a) Explain how Heun's method can lead to a closer approximation of the true solution than Euler's method for solving an ODE IVP. *[(CO4)(Understand/LOCQ)]*

(b) For the equation $\frac{dy}{dt} = f(y,t) = yt^3 - 1.5y$, determine the value of y(1) if y(0) is 1. Use a step size of 0.5. Obtain the solution by i) Euler's method ii) Midpoint method and compare the percentage errors with respect to the exact solution.

[(CO4) (Apply/IOCQ)]

4 + 8 = 12

7. (a) For a system of reactors operating in unsteady state, the material balance equations will be solved by Gauss Jordan method or R K method? Justify. *[(CO4)(Analyse/IOCQ)]*

(b) Water is drained from a vertical cylindrical tank by opening a valve at the base. The rate at which water level drops is given by $\frac{dy}{dt} = -k\sqrt{y}$, where y is the water level in m, t is the time in minutes and k is a constant. If k = 0.06 and the initial water level is 3 m, determine the level of water after 1 minute. Use Heun's method with a step size of 1 minute.

[(CO4) (Apply/LOCQ)]

4 + 8 = 12

Group - E

8. (a) Elaborate Liebmann method to solve elliptical PDE, with no source term for four internal nodes on a 2D geometry.

[(CO5)(Remember/LOCQ)]

(b) For an unsteady state heat conduction problem the equation is given as

$$\frac{\partial T(x,t)}{\partial t} = \frac{\partial^2 T(x,t)}{\partial x^2}$$

$$T(0,t) = 5; T(2,t) = 9 \quad t > 0$$

$$T(x,0) = (4-x)x + 5$$

$$\Delta x = 0.5; \Delta t = 0.5$$

Show the solution matrix as AX=B after applying the implicit scheme for Δt=0.5. *[(CO5)(Analyse/HOCQ)]*

4 + 8 = 12

9. (a) Write down the algorithm for dichotomous search with proper schematic. *[(CO3)(Remember/LOCQ)]*

(b) A firm used lathes, milling machines and grinding machines to produce two machine parts. The following table represents the machining times required for each part, the machining time available on different machines and the profit on each machine part. Find the number of parts 1 and 2 to be manufactured per week to maximize the profit by Simplex method (Show two iterations).

Type of machine	Machining time (mins)		Maximum time available per week (min)
	Part 1	Part 2	
Lathes	12	6	3000
Milling machine	4	10	2000
Grinding machine	2	3	900
Profit per unit	Rs. 40	Rs. 100	

[(CO2)(Analyse/HOCQ)]

(c) What is slack variable? *[(CO2)(Remember/LOCQ)]*

3 + 8 + 1 = 12

Cognition Level	LOCQ	IOCQ	HOCQ
Percentage distribution	30.20	32.30	37.5

Course Outcome (CO):

After the completion of the course students will be able to

1. Given a mathematical problem to be solved numerically, students should be able to identify different computational errors and evaluate them. Students will be able to know how to perform relative and absolute error in each case.
2. Given a linear multivariable problem, students will be able to relate the dependent and independent variables in the appropriate matrix form. Students will be able to identify the broad category of linear algebraic methods to solve the corresponding mathematical problem.
3. Given a non-linear engineering problem requiring single or simultaneous equation, students will be able to select the appropriate numerical algorithm to solve for the unknown variables.
4. Given an engineering problem with time varying solutions, students will be able to select appropriate numerical algorithm (e.g Euler or Runge Kutta method etc.) to determine the dynamic or spatial changes in the dependent variables under given initial/boundary conditions.
5. Given an engineering problem that can be modeled using partial differential equations (PDE), students will be able to identify the type of PDE and its associated boundary conditions. Students will be able to develop the numerical form of the governing equation by applying principles of numerical differentiation.

**LOCQ: Lower Order Cognitive Question; IOCQ: Intermediate Order Cognitive Question; HOCQ: Higher Order Cognitive Question.*