NUMERICAL METHODS IN CHEMICAL ENGINEERING
(CHEN 3104)

Time Allotted : 3 hrs **Full Marks : 70**

Figures out of the right margin indicate full marks.

Candidates are required to answer Group A and any 5 (five) from Group B to E, taking at least one from each group.

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

Group – A
(Multiple Choice Type Questions)

1. Choose the correct alternative for the following: **10 × 1 = 10**

(i) Percentage relative error is given by _____.

(a) $\frac{\text{Approximate Error}}{\text{Current Approximation}} \times 100$ (b) $\frac{\text{True Error}}{\text{Current Approximation}} \times 100$

(c) $\frac{\text{Approximate Error}}{\text{True Value}} \times 100$ (d) $\frac{\text{True Error}}{\text{True Value}} \times 100$

(ii) Order of error for centered difference scheme is _____, where 'h' is the equispaced interval on the independent axis.

(a) O(h) (b) $O(h^2)$ (c) O(1/h) (d) $O(1/h^2)$

(iii) Lagrangian interpolation is primarily arrived through _____ interpolation scheme.

(a) linear (b) nonlinear (c) spline (d) either (a) or (b)

(iv) To evaluate an intermediate value of a dependent variable using quadratic spline technique, the number of equations must be _____, where 'n' is the number of segments considered within the interval.

(a) 2n (b) 5n (c) n (d) 3n

(v) In LU decomposition method to get the solution for a set of simultaneous equations one must factorise the coefficient matrix into _____.

(a) lower and upper triangular matrices (b) lower and diagonal matrices
(c) upper and diagonal matrices (d) lower and inverse of the coefficient matrix

(vi) Diagonally dominant of a coefficient matrix is mandatory with _____.

(a) Gauss Siedel method (b) Gauss Jordon method
(c) Gauss Elimination technique (d) either (a) or (b)

(vii) Newton-Cotes formula is providing an approximation with the integral format as _____, where $f_n(x)$ is an arbitrary polynomial function.

(a) $I = \int_a^b f_n(x)dx, f_n(x) = a_0 + a_1 x + ... + a_n x^n$ (b) $I = \int_a^b f_n(x)dx, f_n(x) = a_0 + a_1(x-a) + ... + a_n(x-a)^n$

(c) $I = \int_a^b f_n(x)dx, f_n(x) = a_0 + a_1(b-x) + ... + a_n(b-x)^n$ (d) $I = \int_a^b f_n(x)dx, f_n(x) = a_0 + a_1\left(x - \frac{a+b}{2}\right) + ... + a_n\left(x - \frac{a+b}{2}\right)^n$

(viii) The equation f(x) is given as $x^3+4x+1=0$. Considering the initial approximation at x=1 then the value of x after first iteration is given as _____ after using Newton Raphson method.
(a) -0.1667 (b) 0 (c) 0.14286 (d) 0.125

(ix) Optimization using Newton's method is primarily to find a solution _____
(a) when f(x) becomes zero (b) when f'(x) becomes zero
(c) both (a) and (b) (d) when f''(x) becomes zero.

(x) Binary conversion of 173 results _____.
(a) 10101101 (b) 11010101 (c) 10111011 (d) 10101011

Group - B

2. (a) What is the difference between chopping and rounding off error? [(CO1)(Remember/LOCQ)]

(b) "True error is always coming up to set up the model accuracy of the process, while approximate error is always coming with the process simulation" – Justify the appropriateness of the statement. [(CO1)(Analyze/IOCQ)]

(c) The derivative of $f(x)=\frac{1}{(1-3x^2)^2}$ is given by $\frac{6x}{(1-3x^2)^2}$. Do you expect to have difficulties evaluating the function at x=0.577 after rounding off 3 digits. [(CO1)(Evaluate/HOCQ)]

2 + 4 + 6 = 12

3. (a) A mass balance for a pollutant in a well-mixed lake can be written as $10^6\frac{dc}{dt}=10^6-10^5c-2{,}50{,}000\sqrt{c}$, where c is the initial concentration of the pollutant with initial guess c = 4 g/m^3. Find out the steady state concentration using Newton-Raphson method (Show three iterations). [(CO3)(Evaluate/HOCQ)]

(b) Consider the function f (x)= $x^3 - 2x + 4$ on the interval [−2, 2] with h = 0.25. Use the forward, and centered finite difference approximations to calculate the second derivatives. [(CO3)(Evaluate/HOCQ)]

8 + 4 = 12

Group - C

4. (a) A civil engineer involved in construction requires 4800, 5800, and 5700 m^3 of sand, fine gravel, and coarse gravel, respectively, for a building project. There are three pits from which these materials can be obtained. The composition of these pits is given by the below table. Outline the augmented form of the matrix in order to obtain the amount in m^3 of the material will be hauled from each of the pits.

	Sand %	Fine Gravel %	Coarse Gravel %
Pit 1	52	30	18
Pit 2	20	50	30
Pit 3	25	20	55

[(CO2)(Evaluate/HOCQ)]

(b) What is the order of truncation error in Trapezoidal and Simpson's 1/3rd rule for integration of a function within the limits? [(CO4)(Remember/LOCQ)]

(c) "One can avoid the back-propagation step when Gauss Jordon method is used to solve simultaneous equations instead of Gauss Elimination method" – Justify the appropriateness of the statement. [(CO2)(Analyze/IOCQ)]

7 + 2 + 3 = 12

5. (a) The amount of mass transported by a pipe over a period of time can be computed using the equation

$$\int_{t_1}^{t_2} Q(t)c(t)dt \quad \text{Where} \quad \begin{matrix} Q(t) = 9 + 4\cos^2(t) \\ c(t) = 5e^{-0.5t} + 2e^{0.15t} \end{matrix}$$

Calculate the total mass flow from 2 mins to 8 mins using trapezoidal rule for integration (h=2 mins). [(CO4)(Evaluate/HOCQ)]

(b) "Iterative method for simultaneous equation solution is much convenient compared to matrix manipulation method" – Justify the appropriateness of the statement. [(CO4)(Analyze/IOCQ)]

(c) "One can use different integration algorithms to find out the area under the function curve with unequal segments." – Justify the appropriateness of the statement. [(CO4)(Analyze/LOCQ)]

6 + 3 + 3 = 12

Group - D

6. (a) What is the purpose of adaptive Runge Kutta algorithm over ordinary Runge Kutta method? [(CO4)(Remember/LOCQ)]

(b) Water is draining out from a cylinder using a valve at the bottom of the tank. The water height in the tank decreases at a rate given by the equation $\frac{dy}{dt} = 0.06\sqrt{y}$. Using Euler's method find out the time required to reach at 85% of the initial height. Use a time step of 0.5 mins. [(CO4)(Evaluate/HOCQ)]

3 + 9 = 12

7. (a) "Heun's method can be approximated as the averaging of the two slopes evaluated at initial and predicted location." – Justify the appropriateness of the statement using proper diagram. [(CO4)(Analyze/LOCQ)]

(b) Compound A diffuses through a 4-cm-long tube and reacts as it diffuses. The equation governing diffusion with reaction is $D\frac{d^2A}{dx^2} - kA = 0$. At one end of the tube, there is a large source of A at a concentration of 0.1 M. At the other end of the tube there is an adsorbent material that quickly absorbs any A, making the concentration 0 M. D = 1.5×10^{-6} cm^2/s; k = 5×10^{-6} s^{-1}. What is the concentration of A as a function of distance in the tube? Use Shooting method and show two iterations. [(CO4)(Evaluate/HOCQ)]

(c) In which type of chemical reaction engineering problem, one should use the shooting method? [(CO4)(Remember/LOCQ)]

3 + 6 + 3 = 12

Group - E

8. (a) Write down 2D PDEs for Laplace equation, Poisson equation and Parabolic equation. [(CO5)(Remember/LOCQ)]

(b) "To provide accuracy, in Crank-Nicolson scheme, difference approximations are developed at the midpoint of the time increment." – Justify the appropriateness of the statement. [(CO5)(Analyze/IOCQ)]

(c) Gas species A is diffusing though a plug flow reactor from x = 0 to x = 10 cm. The concentration of A can be modelled using the following PDE. The superficial velocity vo can be assumed to be 1 cm/s.

$$\frac{\partial C_A}{\partial t} = 0.5\frac{\partial^2 C_A}{\partial x^2} - v_o C_A$$

Subject to the boundary conditions

$$C_A(0,t) = 1$$

$$C_A(10,t) = 0$$

$$C_A(x,0) = 0 \text{ for all } 0 < x < 1$$

Setup the numerical form of the differential equation in form AX = B using an implicit scheme. [(CO5)(Evaluate/HOCQ)]

3 + 4 + 5 = 12

9. (a) Why the Newton's method algorithm for unconstrained optimization problem uses 1st order derivative of the function in contrast to the Newton-Raphson algorithm, although both the algorithm resembles each other? [(CO3)(Understand/LOCQ)]

(b) Use Golden section search to find the maximum value for 'x' in the range [-2,1] for the function $f(x)=-x^4-2x^3-8x^2-5x$. Show 5 iterations. [(CO3)(Evaluate/HOCQ)]

(c) State a significant difference between Fibonacci and Golden section search. [(CO3)(Analyse/IOCQ)]

2 + 8 + 2 = 12

Cognition Level	LOCQ	IOCQ	HOCQ
Percentage distribution	21.88	16.67	61.45

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.