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) The binary conversion of 173 will be _____
(a) 10101101 (b) 11011101 (c) 10111101 (d) 10011101

(ii) Interpolation means _____
(a) only aligning new data points (b) only removing old data points
(c) adding new data points (d) appending new data points

(iii) Truncation error is with the order of _____ for central difference scheme, where 'h' is the step size.
(a) h (b) h2 (c) h3 (d) h4

(iv) The equation f(x) is given as $x^3+4x+1=0$. Considering the initial approximation at x=1 then the value of x1 is given as _____ after using Newton Raphson method
(a) -0.1667 (b) 0 (c) 0.14286 (d) 0.125

(v) The Gauss Jordan method reduces a original matrix into a _____
(a) skew hermitian matrix (b) non-symmetric matrix
(c) identity matrix (d) null matrix

(vi) The value of $\int_{0.2}^{2.2} xe^x dx$ by using one segment trapezoidal rule is _____
(a) 11.672 (b) 11.807 (c) 20.099 (d) 24.119

(vii) Given: $3\frac{dy}{dx}+5y^2=\sin x, y(0)=5$. Applying Euler's method, the value of y(0.3) is _____, when $h=\Delta x=0.3$
(a) -7.5 (b) -6.5 (c) -8.5 (d) -9.5

(viii) For a stable and convergent solution to 1D heat conduction problem with accumulation term the time step must be correlated with the spatial step size as _____, where 'k' is the thermal conductivity of the material.

(a) $\Delta t \geq \frac{1}{2}\frac{(\Delta x)^2}{k}$ (b) $\Delta t \leq \frac{1}{2}\frac{(\Delta x)^2}{k}$ (c) $\Delta t \geq \frac{1}{2}\frac{k}{(\Delta x)^2}$ (d) $\Delta t \leq \frac{1}{2}\frac{k}{(\Delta x)^2}$

(ix) When, applying the Golden Section Search method to a function f(x) to find its maximum, the $f(x_1) > f(x_2)$ condition holds true for the intermediate points x_1 and x_2, in between x_l and x_u. Hence "_____" is the incorrect statement.

(a) the new search engine is determined by $[x_2,x_u]$
(b) the intermediate point x_1 stays as one of the intermediate points
(c) the upper bound x_u remains the same
(d) the new search region is determined by $[x_l,x_1]$

(x) _____ is not a characteristic of the linear programming model

(a) Alternative courses of action
(b) An objective function of maximization type
(c) Limited amount of resources
(d) Non-negativity conditions on the value of decision variables.

Group- B

2. (a) What are rounding and chopping error? Why are they appearing during the application of numerical algorithm? [(CO1) (Remember/LOCQ)]

(b) "Order of truncation error in approximation for Taylor's series is always one less than that of the order of remainder." – Validate the statement. [(CO1) (Evaluate/HOCQ)]

(c) Consider the function $f(x)= x^3 - 2x + 4$ on the interval$[-2, 2]$ with h = 0.25. Use the forward, backward, and centeredfinite difference approximations to calculate the second derivatives. [(CO1) (Apply/IOCQ)]

3 + 3 + (2 + 2 + 2) = 12

3. (a) Derive the algorithm for Secant method and discuss its advantage over the Newton-Raphson method. [(CO3) (Remember/LOCQ)]

(b) "Criterion to understand the condition of a function using condition number does not truly indicate the accuracy of the approximation" – Justify the appropriateness of the statement. [(CO1) (Evaluate/HOCQ)]

(c) In a chemical engineering process, water vapor (H_2O) isheated to sufficiently high temperatures that a significant portionof the water dissociates, or splits apart, to form oxygen (O_2) andhydrogen (H_2):

$$H_2O \Leftrightarrow H_2 + \tfrac{1}{2}O_2$$

If it is assumed that this is the only reaction involved, the molefraction x of H_2O that dissociates can be represented by

$$K = \frac{x}{1-x}\sqrt{\frac{2p_t}{2+x}}$$

Where, K = the reaction equilibrium constant and pt = the totalpressure of the mixture. If p_t = 3.5 atm and K = 0.04, determinethe value of x that satisfies the above equation using bisection method taking lower limit for x is 0 and higher limit for x is 1. Show three iterations. [(CO3)(Apply/IOCQ)]

3 + 3 + 6 = 12

Group - C

4. (a) Elaborate the advantage(s) of LU Decomposition method to solve the linear algebraic simultaneous equations on the basis of a chemical process. [(CO2) (Understand/LOCQ)]

(b) "Over-relaxation parameter multiplied with the current iteration from Gauss-Siedel method reduces the number of iterations to generate the approximate solution of linear algebraic simultaneous equations. However, this relaxation parameter cannot be adjusted in case with Jacobi iteration method." – Justify the appropriateness of the statements. [(CO2) (Evaluate/HOCQ)]

(c) An irreversible, first-order reaction takes place in four well mixed reactors (fig. 1), where reactant A is converted into product B. The rate constant of the reaction is 'k'.The reactors have different volumes and as they are operated at different temperatures, each has a different reaction rate (given in the below table). Develop the augmented matrix to determine the concentration of A and B in each of the reactors at steady state.

Reactor	Volume, V (L)	k, h^{-1}
1	25	0.075
2	75	0.15
3	100	0.4
4	25	0.1

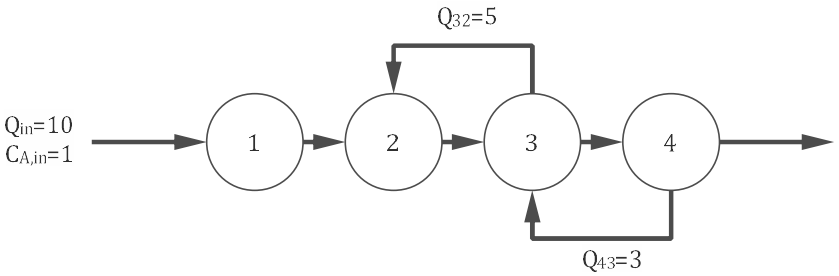

Fig. 1

[(CO2)(Apply/IOCQ)]

3 + (2 + 2) + 5 = 12

5. (a) "If we want to apply Simpson's 1/3rd rule with six data points, we can apply it for the first five data points. While for the rest of the limits, we need to apply Trapezoidal rule" – Elaborate the meaning of the statement based on the order analysis for Simpson's 1/3rd and Trapezoidal rule. [(CO4) (Understand/LOCQ)]

(b) "In trapezoidal rule for integration, the function curve is approximated by a straight line." – Validate the statement. [(CO4) (Evaluate/HOCQ)]

(c) Use Simpson's 1/3rd rule to evaluate the mass leaves a reactor based on the following information.

t, min	0	10	20	30	35	40	45
Q, m^3/min	4.0	4.8	5.2	5.0	4.6	4.3	4.3
C, mg/m^3	10	35	55	52	40	37	32

[(CO4) (Apply/IOCQ)]

3 + 4 + 5 = 12

Group - D

6. (a) During the Runge-Kutta algorithm in order to get a solution for ODE, what is the utility of increment function? [(CO4) (Understand/LOCQ)]

(b) Check using Euler's method, whether the following ODE at y(2) generates stiffness or not? $\frac{dy}{dx} = 0.5x(1-x), y(0) = 2, h = 1$ [(CO4) (Evaluate/HOCQ)]

(c) A mass balance for a chemical in a completely mixed reactorcan be written as $V\frac{dc}{dt} = F - Qc - kVc^2$, where V=12 m^3, c(0)=0 g/m^3, F=175 g/min, k=0.15 m^3/(g)(min). With h=Δt=0.5 min, find out the concentration of the reactant within the reactor at t=1 min using 4th order Runge-Kutta method.

[(CO3)(Analyze/IOCQ)]

3 + 4 + 5 = 12

7. (a) "Heun's method provides better solution for ODE compared to Euler's method" – Justify the appropriateness of the statement in light of mathematical representation for both the algorithms. [(CO4) (Remember/LOCQ)]

(b) "Heun's method algorithm is primarily derived after integrating the function using Trapezoidal rule." – Validate the statement mathematically.

[(CO4) (Evaluate/HOCQ)]

(c) Compound A diffuses through a 4-cm-long tube and reacts asit 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 concentrationof 0.1 M. At the other end of the tube there is an adsorbentmaterial 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) (Apply/IOCQ)]

3 + 4 + 5 = 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) "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) (Evaluate/HOCQ)]

(c) The displacement of a uniform membrane subject to a tension and a uniform pressure can be described by the Poisson equation $\frac{\partial^2 z}{dx^2}+\frac{\partial^2 z}{dy^2}=-\frac{P}{T}$. 1 cm^2membrane that has P/T = 0.6/cm and is fastened so that it has zero displacement along its four boundaries. Find out the coefficient matrix to find the displacement using Liebmann method. [(CO5)(Apply/IOCQ)]

3 + 4 + 5 = 12

9. (a) Through a proper schematic, show that the Golden ratio in Golden Search algorithm for unconstrained optimization problem is given by 0.61803. [(CO3) (Create/HOCQ)]

(b) What are "Slack" variables? What is the importance of these variables in solving linear constrained optimization problem? [(CO2) (Understand/LOCQ)]

(c) A chemical plant makes three major products on a weekly basis. Each of these products requires a certain quantity of raw chemical and different production times, and yields different profits. The pertinent information is in the below table. Note that there is sufficient warehouse space at the plant to store a total of450 kg/week. Set up a linear programming problem to maximize profit.

	Product 1	Product 2	Product 3	Resource Availability
Raw materials (kg/kg)	6	4	12	2500 kg
Production time	0.05 h/kg	0.1 h/kg	0.2 h/kg	55 h/week
Profit	INR 30/kg	INR 30/kg	INR 35/kg	

[(CO2) (Analyse/IOCQ)]

4 + (2 + 1) + 5 = 12

Cognition Level	LOCQ	IOCQ	HOCQ
Percentage distribution	25%	43.75%	31.25%

Course Outcome (CO):

After the completion of the course students will be able to

1. 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. 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. Select the appropriate numerical algorithm to solve for the unknown variables.

4. 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. 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

Department & Section	Submission Link
CHE	https://classroom.google.com/c/NDAwNzk0MzgyMzgz/a/NDU0OTI0MTc4MDY2/details