B.TECH/CHE/5TH SEM/CHEN 3104/2019

NUMERICAL METHODS OF ANALYSIS (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 <u>any 5 (five)</u> from Group B to E, taking <u>at least one</u> 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) Precision ensures
 - (a) the reproducibility of a measurement
 - (b) the closeness of the prediction with the actual
 - (c) the deviation between two successive measurements
 - (d) the average of the successive measurements.
- (ii) The error with the trapezoidal integration ______ compared to Simpson's 1/3 rd rule, when the function is a polynomial one.
 (a) is less
 (b) is more
 (c) is same as
 (d) can't be
- (iii) LU decomposition of a matrix gives rise to
 - (a) a diagonal matrix
 - (b) lower triangular matrix
 - (c) upper triangular matrix
 - (d) both lower and upper triangular matrix.
- (iv) The PDE given by $x \frac{d^2y}{dx^2} + y \frac{dy}{dx} + 10y = 0$
 - (a) is linear w.r.t the dependent variable
 - (b) is nonlinear w.r.t the dependent variable
 - (c) is linear w.r.t independent variable
 - (d) is nonlinear w.r.t the independent variable.
- (v) A 2×2 system of equations is given by $\begin{bmatrix} 0.01 & 10 \\ 1 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 3 \\ 5 \end{bmatrix}$ is ill-conditioned.

To solve the system, an operation needs to be done first. The operation can be (a) Pivoting (b) Column exchange (c) Scaling (d) None of (a), (b), (c).

B.TECH/CHE/5TH SEM/CHEN 3104/2019

- (vi) A condition for Gauss-Siedel method to converge iteratively is
 - (a) diagonal terms should be non-zero
 - (b) diagonal terms greater than the maximum of the off-diagonal terms
 - (c) diagonal terms greater than the sum of the off-diagonal terms
 - (d) no off-diagonal terms to be present.
- (vii) The Euclidean norm of a vector <u>x</u> with n components is
 - (a) dependent on the magnitude of each component
 - (b) is dependent on the direction of \underline{x}
 - (c) dependent on the square of each component
 - (d) none of the above.

(viii) In the generic PDE given by $A \frac{\partial^2 T}{\partial x^2} + B \frac{\partial^2 T}{\partial y \partial x} + C \frac{\partial^2 T}{\partial y^2} + D = 0$ the equation is elliptic if B² - 4AC is

(a) = 0 (b) > 0 (c) < 0 (d) =1.

- (ix) Two point boundary value problems usually contain
 - (a) conditions specified at the initial point
 - (b) conditions specified at two boundary points
 - (c) two conditions specified at one boundary point
 - (d) two initial conditions specified at one boundary point.
- (x) The backward difference approximation for the derivative of a function is (a) $\vartheta(h)$ accurate (b) $\vartheta(h^2)$ accurate (c) $\vartheta(\sqrt{h})$ accurate (d) not dependent on h.

Group – B

2. (a) Manning's formula for a rectangular channel can be written as

$$Q = \left(\frac{1}{n}\right) \frac{\left(BH\right)^{\frac{5}{3}}}{\left(B + 2H\right)^{\frac{2}{3}}} \sqrt{s}$$

B: width = 20 m; H:depth = 0.3 m; Q is the flow m^3/s ; n:roughness coefficient and s: slope within the channel.

Roughness and slope are to only a $\pm 10\%$ precision. Roughness is about 0.03 with a range from 0.027 to 0.033. Slope is about 0.0003 with a range from 0.00027 to 0.00033. Using first order error analysis, determine the sensitivity of the flow prediction with the formula against those two parameters.

(b) "With the step size the round-off error gets decreased." - Justify the correctness of the statement.

9 + 3 = 12

B.TECH/CHE/5TH SEM/CHEN 3104/2019

$$\frac{\partial T}{\partial t} = 0.5 \frac{\partial^2 T}{\partial x^2} + q$$

Subject to the boundary conditions
T(0,t)=100
T(10,t)=50

T(10,t) = 50

T(x,0)=0 for all 0 < x < 10

Choose 3 internal grid points and solve for 2 timesteps with a step size of 0.5. Choose explicit scheme.

(b) If the right hand side boundary condition in the above problem were changed to $\kappa \frac{\partial T}{\partial x}\Big|_{(10,1)} = 4$ where $\kappa = 3.85$ W/cm K, show numerically how the temperature T(10,t) can be evaluated.

8 + 4 = 12

9. (a) Solve the following PDE

 $\frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{\partial t}$, T(1,t) = 1, T(0,t) = 0.5 and initial condition, T(x,0) = 0, 0 < x < 1Use Crank-Nicholson finite difference scheme to solve for three internal grid points. Take two timesteps each of 0.1.

(b) Solve the problem in (a) using Euler explicit and compare the result.

8 + 4 = 12

B.TECH/CHE/5TH SEM/CHEN 3104/2019

3. The outflow concentration from a reactor is measured at a number of times over a 24-hr period:

| t, h | 0 | 1 | 5.5 | 10 | 12 | 14 | 16 | 18 | 20 | 24 |
|---------|---|-----|-----|-----|----|----|-----|----|----|-----|
| C, mg/L | 1 | 1.5 | 2.3 | 2.1 | 4 | 5 | 5.5 | 5 | 3 | 1.2 |

The flow rate for the outflow in m³/s can be computed with the following equation:

$$Q(t) = 20 + 10 sin\left(\frac{2\pi}{24}(t-10)\right)$$

Using Simpson's 1/3rd rule find out the flow weighted average concentration leaving the reactor over the 24 \mbox{h}

$$\overline{c} = \frac{\int_{o}^{t} Q(t)c(t)dt}{\int_{o}^{t} Q(t)dt}$$

Group – C

4. (a) The volume V of a torus-shaped water tube is given by:



(b) Determine r_1 if $V=2500 \text{ m}^3$ and $r_2=18\text{m}$. Use bisection method. Find the solution of equation $\frac{1}{x}-2=0$ by using Newton's method. Choose the initial guess of x to be 1.4. Does the solution converge? If not, explain the reason with a graph. 7+5=12

5. (a) The linear system is given by
$$Ax = b$$
 where $A = \begin{bmatrix} 4 & 5 & -2 \\ 2 & -5 & 2 \\ 6 & 2 & 4 \end{bmatrix}$ and $\underline{x} = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix}$ and

 $\underline{b} = \begin{vmatrix} -6\\ 24\\ 30 \end{vmatrix}$

- (i) Check whether the system can be solved by Gauss-Siedel by using the concept of diagonal dominance.
- (ii) If yes, then use Gauss-Siedel. If no, then use an alternate technique.

CHEN 3104

3

B.TECH/CHE/5TH SEM/CHEN 3104/2019

(b) The van der Waals equation gives a relationship between the pressure P (in atm.), volume V (in L), and temperature T (in K) for a real gas:

$$P = \frac{nRT}{V - nb} - \frac{n^2a}{V^2}$$

where n is the number of moles, R = 0.08206 (L atm)/(mole K) is the gas constant, and a (in L² atm/mole²) and b (in L/mole) are material constants. Consider 1.5 moles of nitrogen (a = 1.39 L^2 atm/mole², b = 0.03913 L/mole) at 25°C stored in a pressure vessel. Determine the volume of the vessel if the pressure is 13.5 atm. Use Newton-Raphson method to solve the system. 6 + 6 = 12

Group – D

A chemical compound decays over time when exposed to air and can be modelled using the equation given below:

$$\frac{dn}{dt} = -0.8n^{3/2} + 10n_0(1 - e^{-3t})$$

Solve the equation using 2^{nd} order RK method to find the concentration n at 0.4s using a time step of 0.2s. The initial concentration n_o is 2000. Use Euler implicit method.

(b) A function f(x) is expanded about a point, x_i using Taylor series to obtain and expression for $f(x_{i+1})$. Derive the expression for the numerical approximation of $\frac{df}{dx}\Big|_{x=x_i}$ using central difference scheme. Also determine the order of accuracy.

- 7. (a) Consider the following system of ODEs $\frac{dx}{dt} = 2x + 2y \text{ and } \frac{dy}{dt} = 2x - y \text{ from } t = 0 \text{ to } t = 1.0$ x(0) = 1 and y(0) = 2Chose step size of h = 0.5 and use any predictor-corrector method.
 - (b) Use Taylor series to linearize e^{-3t} to the 1st order approximation and evaluate the value of t = 1 based on expansion around t = 0. Compare with the true solution and evaluate the global truncation error.

8 + 4 = 12

Group – E

- 8. (a) The temperature of a cylindrical rod of length 10cm follows the governing given below. The rod is heated at the point, 4cm from the left end through a laser torch at the rate of 2 W/cm³.
- CHEN 3104

6. (a)

12

4