NUMERICAL METHODS IN CHEMICAL ENGINEERING
(CHE3101)

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

(ii) The Newton-Raphson method of finding roots of nonlinear equations falls under the category of _____.
(a) open (b) random (c) graphical (d) bracketing

(iii) Precision refers to how closely _____.
(a) individual computed or measured values agree with each other
(b) individual computed or measured values agree with true value
(c) approximate values agree with each other
(d) approximate values agree with true value

(iv) 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

(v) With the numerical integration using Simpson's 1/3rd rule the order of truncation error is _____, where 'h' is equispaced intervals on independent axis.
(a) h^4 (b) h^3 (c) h^5 (d) h^6

(vi) Unsteady heat conduction in a thin circular rod, the ends of which are kept at two different temperatures give rise to _____.
(a) initial value problems (b) partial differential equations
(c) boundary value problem (d) first order ODE

(vii) Initial value problems with 2 dependent variable solved by 4th order RungeKutta method require the calculation of _____ slopes at each time step.
(a) 4 (b) 2 (c) 8 (d) 6

(viii) A first order ordinary differential equation must contain at least the _____.
(a) second derivative of the dependent variable
(b) first derivative of the dependent variable
(c) square of the first derivative of the dependent variable
(d) first derivative of the independent variable

(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) The partial differential equation $5\frac{\partial^2 z}{\partial x^2}+6\frac{\partial^2 z}{\partial y^2}=xy$ is classified as _____
(a) elliptic (b) Laplace equation (c) Poisson equation (d) both (a) and (c)

Fill in the blanks with the correct word

(xi) During quadratic spline with 'n' data points number of unknowns will be equal to _____.

(xii) The value of $\int_{0.2}^{2.2} xe^x dx$ by using one segment trapezoidal rule is _____.

(xiii) The order of convergence for Newton-Raphson method is equal to _____.

(xiv) Gauss Elimination method yields _____ matrix.

(xv) 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.

Group - B

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

T°C	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°C using Newton's backward difference interpolation scheme. *[(CO2)(Analyse/HOCQ)]*

(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) Elaborate on Newton-Raphson and Secant method with a schematic representation of the iteration. *[(CO3)(Remember/LOCQ)]*

6 + 3 + 3 = 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)(Evaluate/HOCQ)]

(b) In between Newton's method and fixed point iteration method, which method will provide less number of iterations to evaluate a root of a nonlinear equation and why? *[(CO3)(Remember/LOCQ)]*

8 + 4 = 12

Group - C

4. (a) "One can use different integration algorithms to find out the area under the function curve with unequal segments." – Justify the appropriateness of the statement. *[(CO5)(Remember/LOCQ)]*

(b) "Gauss Siedel is faster than that of the Jacobi iteration method" – Justify the appropriateness of the statement. *[(CO3)(Analyze/IOCQ)]*

(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

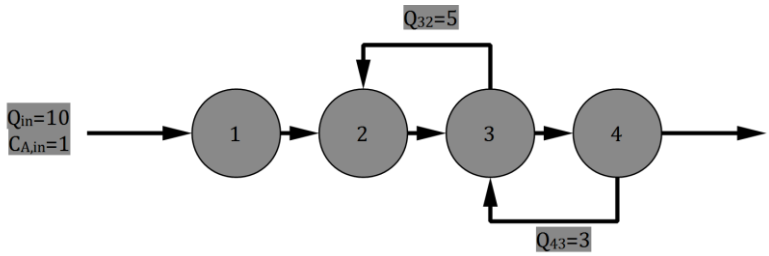

Fig. 1

[(CO3)(Evaluate/HOCQ)]

2 + 3 + 7 = 12

5. (a) How do we integrate a function with the limits using Trapezoidal rule? Explain with a diagram. *[(CO5)(Remember/LOCQ)]*

(b) Use Simpson's 1/3rd rule to evaluate the mass leaves a reactor based on the following information. *[(CO5)(Evaluate/HOCQ)]*

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

2 + 10 = 12

Group - D

6. (a) Prove that for forward difference method, the local truncation error $e_i^{TR} = O(h)$, where *h* is the grid size in space. *[(CO1)(Understand/LOCQ)]*

(b) Given the boundary value problem $\frac{d^2y}{dx^2} - 2\frac{dy}{dx} + y = 0$, with $\left.\frac{dy}{dx}\right|_{x=1} = 5$ and y(1) = 2. Discretize the problem using second-order accurate central differences for

the derivatives and backward difference derivative for the boundary condition at x = l for a constant step size h. *[(CO4)(Evaluate/HOCQ)]*

(c) What are the differences between global and local truncation error? State with example. *[(CO1)(Remember/LOCQ)]*

4 + 4 + 4= 12

7. (a) For the ordinary differential equation given by $\frac{dy}{dx} = -1.2y + 7e^{-0.3x}$ with initial condition of y(0) = 3, find out the value of y(0.5) using 3rd order RK method. Use a step size of h= 0.5. *[(CO4)(Apply/IOCQ)]*

(b) The local truncation error in 3rd order RK method is $O(h^3)$. Starting with h = 0.5, explain what would happen if h is reduced to 0.05. *[(CO1,CO4)(Analyse/HOCQ)]*

(c) If there are two ODEs with two initial conditions, how many slopes are required to be evaluated when 2nd order RK method is used and why? *[(CO4)(Remember/LOCQ)]*

6 + 4 + 2 = 12

Group - E

8. (a) "Implicit scheme to solve PDE is an iterative process, while explicit scheme is a matrix manipulation process" – Justify the appropriateness of the statement. *[(CO4)(Apply/IOCQ)]*

(b) "Navier Stokes unsteady state equations in Cartesian coordinate system have both Laplacian and parabolic term." – Justify the appropriateness of the statement. *[(CO4)(Apply/IOCQ)]*

(c) The temperature distribution in a long thin rod of length 10cm is governed by the equation:

$$\alpha \frac{\partial^2 T}{\partial x^2} = \frac{\partial T}{dt}$$

The thermal diffusivity = 0.835 cm^2/s. The rod is divided into nodes equally spaced at 2cm interval for finite differencing. The left end of the rod is kept at 80°C and the other end at 20°C. With a time step size of 0.1s, formulate the tri-diagonal matrix after applying Crank-Nicolson scheme. *[(CO4)(Evaluate/HOCQ)]*

3 + 3 + 6 = 12

9. (a) Write down the algorithm for dichotomous search with proper schematic. *[(CO6)(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). *[(CO6)(Analyse/HOCQ)]*

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	

4 + 8 = 12

Cognition Level	LOCQ	IOCQ	HOCQ
Percentage distribution	26.04	18.75	55.21