Name: **Enrolment No:**	UPES University of Tomorrow

UPES
End Semester Examination, May 2025

Programme Name : B. Tech Chemical Engineering **Semester : IV**
Course Name : Numerical Methods in ChE **Time : 03 hrs**
Course Code : CHCE2019 **Max. Marks: 100**
Nos. of page(s) : 2
Instructions: (a) Attempt all questions.
(b)Assume the value of missing data, if any.

SECTION A
(12×5 = 60 M)

S. No.		Marks	CO
Q 1	In the below system of linear equations assume any real value of a_{12}, a_{23}, a_{31} and b_2 so that the system has a unique solution and solve the equation by Gauss Gauss-Seidel method $\begin{bmatrix} a_{12} & 2 & 1 \\ 1 & 3 & a_{23} \\ a_{31} & 2 & 6 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2 \\ b_2 \\ 3 \end{bmatrix}$	**12 M**	**CO1**
Q 2	The Ergun equation is used to describe the flow of fluid through a packed bed. ΔP is the pressure drop, ρ is the density of the fluid , G_o is the mass velocity, D_P is the diameter of the particles within the bed, μ is the fluid viscosity, L is the length of the bed and ε is the void fraction of the bed. $$\frac{\Delta P \rho D_P}{G_o^2 L}\frac{\varepsilon^3}{1-\varepsilon} - 150\frac{1-\varepsilon}{\left(D_P G_o / \mu\right)} - 1.75 = 0$$ Experiments are carried out on a packed bed to estimate the void fraction of the bed, ε. The best fit values of the dimensionless parameters of the bed are reported as, $\frac{D_P G_o}{\mu} = 1000$ and $\frac{\Delta P \rho D_P}{G_o^2 L} = 10$. Use an open iterative scheme of your choice to estimate the value of ε using an initial guess of 0.25. Do *Three* iterations.	**12 M**	**CO2**
Q 3	Heat transfer in a straight fin of uniform cross section is given as, $$\frac{d^2\theta}{dx^2} - m^2\theta = 0$$ $x=0, \quad \theta = 1$	**12 M**	**CO3**

	$x=1, \quad \frac{d\theta}{dx} = -(Bi)\theta$ Where θ is the dimensionless temperature at any position in the fin, x is the dimensionless location, Bi is the dimensionless Biot number, and m^2 is the product of Bi and a dimensionless group involving the fin dimensions. Obtain the algebraic equations to be solved using the finite difference technique with step size 0.25. [You don't need to solve the problem]		
Q 4	Fit a second-order polynomial using the least square method to the following data x: 0, 1, 2, 3, 4, 5 y: 2.1, 7.7, 13.6, 27.2, 40.9, 61.1	**12 M**	**CO2**
Q5	The river is 80 meters wide. The following table gives the depth D in meters at a distance x meters from one bank. Calculate the cross-section area of the river using (a) Simpson's 1/3 rule (b) Simpson's 3/8 rule. *x* in meter: 0, 10, 20, 30, 40, 50, 60, 70, 80 *D* in meter: 0, 4, 7, 9, 12, 15, 14, 8, 3	**12 M**	**CO3**

Q 4 data:

x	0	1	2	3	4	5
y	2.1	7.7	13.6	27.2	40.9	61.1

Q5 data:

x in meter	0	10	20	30	40	50	60	70	80
D in meter	0	4	7	9	12	15	14	8	3

SECTION B
(20×2 = 40 M)

Q 6	(a) Use the Newton-Raphson method, with 3 as starting point, to find a fraction that is within 10^{-4} of $\sqrt{10}$. (b) Discuss the conditions for the rate of convergence of the Newton-Raphson algorithm using the fixed-point iteration method.	**20 M**	**CO2**
Q 7	Consider a series reaction $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ carried out in a batch reactor. The differential equation for component A is, $\frac{dC_A}{dt} = -k_1 C_A$ for component B is,	**20 M**	**CO4**

	$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B$$ and for component C , $$\frac{dC_c}{dt} = k_2 C_B$$ The initial condition is: at t =0, $C_A = 1, C_B = 0$, and $C_c = 0.5$. The rate constants are $k_1 = k_2 = 1\,\text{sec}^{-1}$. Use the fourth-order Runge-Kutta method to determine the concentration of A, B and C up to 6 sec, using a step size of 2 sec.		