Ref. No. : Ex/Che/PC/B/T/221/2023

B.E. CHEMICAL ENGINEERING SECOND YEAR SECOND SEMESTER – 2023
NUMERICAL ANALYSIS FOR CHEMICAL ENGINEERS

Time: 3 hrs **Full Marks: 100**

Part I

Use separate answer scripts for each part

All questions carry equal marks

(Answer any <u>five</u> questions)

1. The following system of equations is designed to determine concentrations (the c's in g/m^3) in a series of coupled reactors as a function of amount of mass input to each reactor (the right-hand sides in g/d),

$$15c_1 - 3c_2 - c_3 = 3300$$
$$-3c_1 + 18c_2 - 6c_3 = 1200$$
$$-4c_1 - c_2 + 12c_3 = 2400$$

Solve this problem with the Gauss-Seidel method to $\varepsilon_s = 5\%$

2. Solve the following nonlinear equations by multi-dimensional Newton Raphson method:

$$f(x,y) = xy^2 + 3x + 4y^2 = 3$$

$$f(x,y) = 2x^2 - 6y^2 + x^2y = 7$$

Consider the initial guess as $x^T = [1,1]$, perform three iterations.

3. Use classical Runge-Kutta method of fourth order to find the numerical solutions at $x = 0.4$ for $\frac{dy}{dx} = \sqrt{x+y}$, y (0.4) =0.41, Assume step length h= 0.25, compare the results with analytical solution. [For analytical solution, consider $z^2 = x + y$]

4. Consider the ODE $\begin{bmatrix} y_1' \\ y_2' \end{bmatrix} = \begin{bmatrix} -100 & 0 \\ 2 & -1 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}$ with $y_0 = [2 \quad 1]^T$. Use explicit Euler technique with h=0.02 to obtain y (t_1=0.01). Integrate the ODE (h=0.02). Compare the results and comment.

5. Solve $\frac{dy}{dt} = ye^{-4}$ with y = 1 at t = 0 and compute y at t = 3 using 4th order Adams-Bashforth method (h=0.5).

6. Solve using SOR (successive over relaxation) with $\omega = 1.5$. Carry out 3 iterations starting with $x^{(1)} = [1 \quad 2 \cdot \quad 1]^T$,

$$\begin{bmatrix} 2 & 1 & 0 \\ 1 & 2 & 1 \\ 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 4 \end{bmatrix}$$

7. Use the finite difference approach to solve the following equation for a 10 m rod with $h' = 0.01\ m^{-2}$, T_a=20 and the boundary conditions, T(0) =40, T(10) = 200.

$$\frac{d^2T}{dx^2} + h'(T_a - T) = 0$$

[Turn over

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Time: 3 hrs **Full Marks: 100**

PART - II (50 marks)

Use separate answer scripts for each part

Answer any five questions

All question carry equal marks

1. The Michaelis–Menten equation occurs in Chemical Kinetics and has the form

$$v(x)=\frac{ax}{b+x}$$

Determine the coefficients a and b using linear least square approximation to the following data obtained in an experiment to measure velocity (v) of an enzymed–catalysed reaction at various concentrations (x). See table below

Velocity, v	0.197	0.139	0.068	0.0427	0.027	0.015
Concentration, x	21.5	21.0	19.0	16.5	14.5	11.0

2. Find the Newton's divided difference interpolating polynomial for the function $f(x)$ using the following data and, hence find $f(1)$.

x	-1	0	3	6	7
$y=f(x)$	3	-6	39	822	1611

3. Find $f(5)$ using Lagrange's formula through the following set of data points.

x	1	2	7	8
$f(x)$	4	5	5	4

4. Consider the following data table to find an interpolating polynomial using Newton's forward difference formula. Also find $f(0.5)$.

x	-2	-1	0	1	2	3
$f(x)$	15	5	1	3	11	25

5. Consider the following data table to find $f'(30)$.

x	0.5	1.0	1.5	2.0	2.5	3.0
$f(x)$	-0.347	0.000	0.608	1.386	2.291	3.296

6. Compute the integral integration, $I=\int_0^1 \frac{5x}{5+x}dx$ using both Trapezium and Simpson's 1/3 rules, taking $h = 0.1$.