

X/K/TY

Reg. No:



VIT

Vellore Institute of Technology

Final Assessment Test – November 2025

Course: BCHE201L

Computational Methods in Chemical Engineering

Class NBR(s): 1221 / 1225

Time: Three Hours

Slot: C2+TC2

Max. Marks: 100

- KEEPING MOBILE PHONE/ANY ELECTRONIC GADGETS, EVEN IN 'OFF' POSITION IS TREATED AS EXAM MALPRACTICE
- DON'T WRITE ANYTHING ON THE QUESTION PAPER

COs	CO Statements
CO1	Formulate mathematical model to solve engineering problems using numerical methods.
CO2	Solve roots of a single and simultaneous equation using numerical methods
CO3	Select suitable numerical regression and interpolation techniques for data analysis
CO4	Compute numerical integration and optimization
CO5	Determine the numerical solution for ordinary and partial differential equations

BL – Blooms Taxonomy Level (1 – Remember, 2 – Understand, 3 – Apply, 4 – Analyse, 5 – Evaluate, 6 – Create)

Answer ALL Questions
(10 X 10 = 100 Marks)

- Given that the equation $x^{2.2} = 69$ has a root between 5 and 8. Use the method of regula falsi to determine it up to three significant digits. CO1 BL3
- Use Newton-Raphson method to find a real root of the equation $xe^x = 1$ using starting value $x_0=1$ upto three significant digits. CO2 BL3
- Use Gauss elimination method to solve the following system of equations. CO2 BL3

$$\begin{aligned} 10x_1 - x_2 + 2x_3 &= 4 \\ x_1 + 10x_2 - x_3 &= 3 \\ 2x_1 + 3x_2 + 20x_3 &= 7 \end{aligned}$$
- Construct divided difference table for the data given below: CO3 BL3

x	0.5	1.5	3.0	5.0	6.5	8.0
f(x)	1.625	5.875	31.0	131.0	282.125	521.0

Hence, find the approximation to the value of f(7).
- Find the maximum of $f(x) = 2x - 1.75x^2 + 1.1x^3 - 0.25x^4$ using Golden section search ($a = -2$, $b = 4$). Carry out three steps. CO4 BL3
- Maximize using simplex method: $Z = 7x_1 + 6x_2$ Subject to: CO4 BL3

$$\begin{aligned} x_1 + x_2 &\leq 4 \\ 2x_1 + x_2 &\leq 6 \\ x_1, x_2 &\geq 0 \end{aligned}$$

7. Find the approximate value of

$$I = \int_0^1 \frac{dx}{1+x}$$

By single application of (i) trapezoidal rule, (ii) Simpson's $1/3^{\text{rd}}$ rule and (iii) Simpson's $3/8^{\text{th}}$ rule. The exact solution is $I = \ln 2 = 0.693147$ correct to six decimal places.

8.

Use the multiple application of Simpson's $1/3^{\text{rd}}$ rule with $n=4$ to estimate the integral of

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

From $a=0$ to $b=0.8$. Recall that the exact integral is 1.640533. Compute the true error percentage.

CO5 BL3

9.a)

Use Euler's method to numerically integrate:

$$\frac{dy}{dx} = -2x^3 + 12x^2 - 20x + 8.5$$

From $x=0$ to $x=2$ with a step size of 0.5. The initial condition at $x=0$ is $y=1$.

CO5 BL3

OR

9.b)

Use the midpoint method to numerically integrate

$$\frac{dy}{dx} = -2x^3 + 12x^2 - 20x + 8.5$$

From $x=0$ to $x=2$ using a step size of 0.5. The initial condition at $x=0$ is $y=1$.

CO5 BL3

10.a)

Differentiate between elliptic, parabolic and hyperbolic partial differential equations giving examples of each. Differentiate amongst Dirichlet, Neumann and Robin-type boundary conditions.

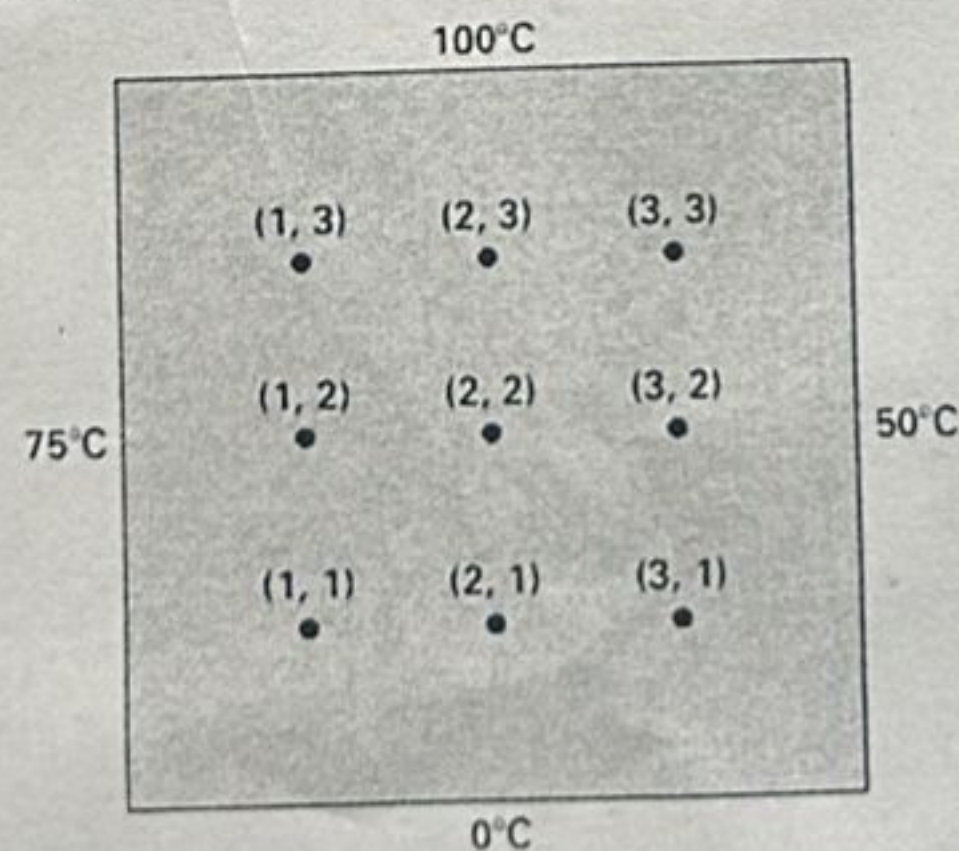
CO5 BL2

OR

10.b)

Use Liebmann's method (Gauss-Siedel) to solve for the temperature of the heated plate (modelled by the Laplacian equation) shown in Figure below. Employ overrelaxation with a value of 1.5 for the weighting factor and perform one iteration.

CO5 BL3



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