VIT
Vellore Institute of Technology

Final Assessment Test – November 2025

Course: BCHE201L - Computational Methods in Chemical Engineering

Class NBR(s): 1219 / 1223

Slot: D1+TD1

Time: Three Hours

Max. Marks: 100

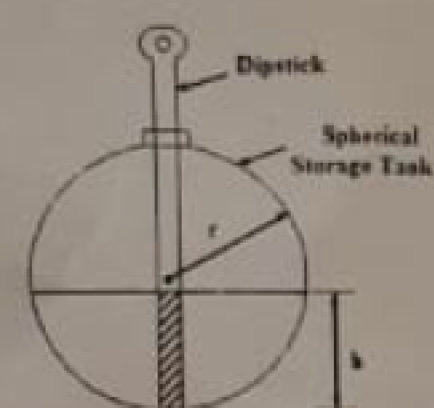
- KEEPING MOBILE PHONE/ANY ELECTRONIC GADGETS, EVEN IN 'OFF' POSITION IS TREATED AS EXAM MALPRACTICE
- DON'T WRITE ANYTHING ON THE QUESTION PAPER

COs	CO Statements
CO1	Formulate mathematical model for solving engineering problems using computational methods.
CO2	Solve roots of a single and simultaneous equation using computational 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)

1. A spherical storage tank containing oil is attached with a dipstick of 16 ft long as shown in the Figure. CO1 BL3



The relationship between the volume, height and radius is given by the following general equation

$$V = \pi h^2 \left[\frac{3r - h}{3}\right]$$

Apply Secant method to determine the height, h, to which the dipstick is wet with oil. Take the initial guess values for height as 3 and 4 ft.

Data: Radius, r = 6 ft and volume, V = 800 ft^3. Specified error, $\varepsilon_s = 0.1\%$.

2. Schematic of a separation system consisting of two flash tanks in series and the experimental data are available for streams F, V_1, V_2, and L_2, as shown in Table. CO2 BL3

Component	Mass Fraction			
	F	V_1	V_2	L_2
Methanol	0.3	0.68	0.44	0.04
Ethanol	0.4	0.27	0.55	0.35
Butanol	0.3	0.05	0.01	0.62

The feed rate, F, is 1000 kg/min. Write mass balances on each of the three components using the supplied data. Determine the flowrates, V_1, V_2, and L_2, using Gauss Seidel method.

3. The following data define the sea-level concentration of dissolved oxygen (O) for fresh water as a function of temperature (T). CO3 BL3

T, (°C)	0	8	16	24	32
O, (mg/L)	14.62	11.84	9.88	8.42	7.31

Apply Lagrangian interpolating polynomial to determine the concentration of dissolved oxygen at 26°C.

4. Given a set of experimental data points for the equilibrium concentration of an adsorbate in the solid phase (q_e) and the equilibrium concentration in the liquid phase (C_e), use a linear regression method to determine the Freundlich constants, (k) and (1/n). CO3 BL3

C_e, (g/L)	30	68	157	250	346	446
q_e, (mg/g)	68	96	150	186	198	205

Note: The non-linear form of the Freundlich isotherm is $q_e = kC_e^{1/n}$.

5. In a process plant, a centrifugal pump is tested to determine its efficiency as a function of volumetric flow rate Q (m^3/h). The efficiency (%) is modeled by a cubic polynomial equation. CO4 BL3

$$\eta(Q)\% = 0.0071Q^3 - 0.3996Q^2 + 6.0829Q - 2.8411$$

Determine the volumetric flow rate, Q, at which the maximum efficiency, η, of the pump is achieved using Newton's optimization. Take initial guess for efficiency, η, as 20 and the specified error, $\varepsilon_s = 1\%$.

6. A company makes two types of products, A and B. These products are produced during a 40 hour work week and then shipped out at the end of the week. Profit per tonne and resource usage per tonne of products are given below. CO4 BL3

Resource	Product A	Product B	Resource Availability
Raw materials (kg /kg)	20	5	10000
Production time (h/tonne)	0.04	0.12	40
Profit ($/tonne)	3600	1600	

Develop a linear program to maximize the profit using SIMPLEX method.

7. 60 mol % n-heptane (A), 40 mol % n-octane (B)] were subjected to a differential distillation at atmospheric pressure. The mole fraction data and the required information is given in the following Table. Compute the moles of distillate and residue using multiple application trapezoidal and Simpson's 3/8th numerical integration method. Basis: F = 100 mol, x_F = 0.60, x_w = 0.30. CO4 BL3

x	0.30	0.40	0.50	0.60
y^*	0.48	0.61	0.68	0.76
$1/(y^*-x)$	5.56	4.76	5.56	6.25

For distillation of binary mixture, the amount of residue is identified using Rayleigh equation and is given below.

$$\ln\frac{F}{W} = \int_{x_W}^{x_F} \frac{dx}{y^* - x}$$

8. A mass balance for a chemical in a completely mixed reactor can be written as CO5 BL3

$$V dC_{out}/dt = QC_{in} - QC_{out}$$

If $C_{in} = C_b(1 - e^{-0.12t})$, calculate the outflow concentration of a conservative substance (no reaction) for a single, completely mixed reactor as a function of time.

Employ values of C_b=40 mg/m³, Q=6 m³/min, V=100 m³, and C_0=20 mg/m³. Apply Runge-Kutta 4th order method to compute the outlet concentration, C_{out}, from t=0 to 15 min using Δt = 5 min.

Note: C_0 is the initial concentration. i.e $C_{out}(0) = C_0$.

9.a) Compound A diffuses through a 10 cm long tube and reacts as it diffuses. The following governing equation for diffusion with reaction is considered. CO5 BL3

$$D\frac{d^2A}{dx^2} - kA = 0$$

At one end of the tube, there is a large source of A at a concentration of 1M. At the other end of the tube there is an adsorbent material that quickly absorbs any A, making the concentration 0 M. If D=1.5×10⁻⁶ cm²/s and k=5×10⁻⁶ s⁻¹. Apply suitable computational method to determine the concentration of A as a function of distance in the tube. Take Δx = 2.5 cm, initial guesses as ones and specified error, ε_s = 0.5%.

OR

9.b) A steady-state heat balance for a 10-m rod is given by the following equation. CO5 BL3

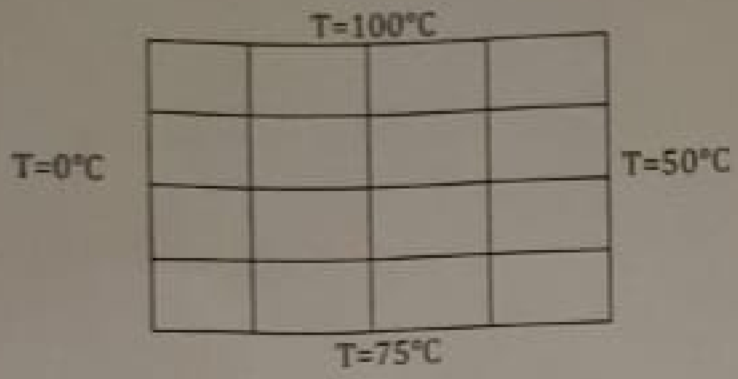
$$\frac{d^2T}{dx^2} - 0.2T = 0$$

Apply suitable computational method to determine the temperature of the rod as a function of temperature. Take Δx = 2.5 m, initial guesses as ones and specified error, ε_s = 1%. Boundary conditions: T(0) = 240°C and T(10) = 150°C.

10.a)	Apply suitable PDE solving method to compute the steady-state distribution of temperature of the heated plate of size 4 ft × 4 ft as shown in Figure.	CO5	BL3

The temperature distribution is given by the following Laplace equation.

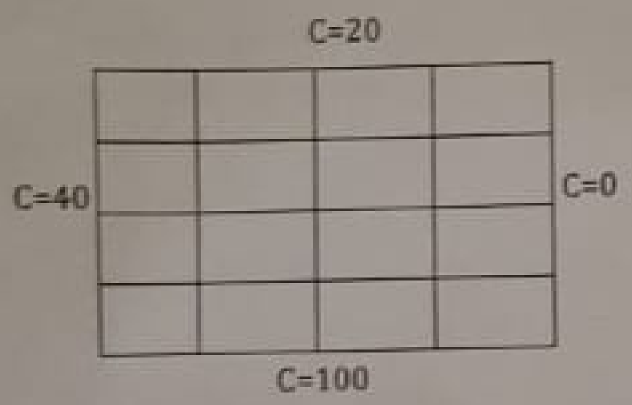
$$\frac{d^2T}{dx^2} + \frac{d^2T}{dy^2} = 0$$



Note: Solve only for 2 iterations. Take all initial or starting guesses as zero.

OR

10.b)	Apply suitable PDE solving method to compute the steady-state distribution of concentration for the 4 ft × 4 ft tank as shown in Figure.	CO5	BL3



The PDE governing this system is

$$D\left(\frac{d^2C}{dx^2} + \frac{d^2C}{dy^2}\right) - kC = 0$$

Data: $D = 0.5$; $k = 0.1$. Take $\Delta x = \Delta y = 1$ ft.

Note: Solve only for 2 iterations. Take all initial or starting guesses as zero.

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