

BIRLA INSTITUTE OF TECHNOLOGY & SCIENCE, PILANI

Numerical Methods for Chemical Engineers (CHE F242) – Comprehensive Examination

Date - 06/05/2023

Part – I (Closed Book)

Maximum Marks - 80

1. Explain the significance of condition number value for a function. Compute the condition number of the function $f(x) = \sqrt{x^2 - 1} - x$ for $x = 300$. [2+9]
2. Using Secant method, determine the value of x if $x^3 = 20$. Take $x_0 = 4$, $x_1 = 5.5$ and perform three iterations. [9]
3. Nitrogen gas follows the ideal gas law $pV = nRT$ where n is the number of moles and T is the absolute temperature. The following pressure – temperature data were obtained for $V = 10 \text{ m}^3$ and a mass of 1 kg nitrogen (molecular weight 28)

T (°C)	-40	0	40	80	120	160
p (N/m ²)	6900	8100	9300	10500	11700	12900

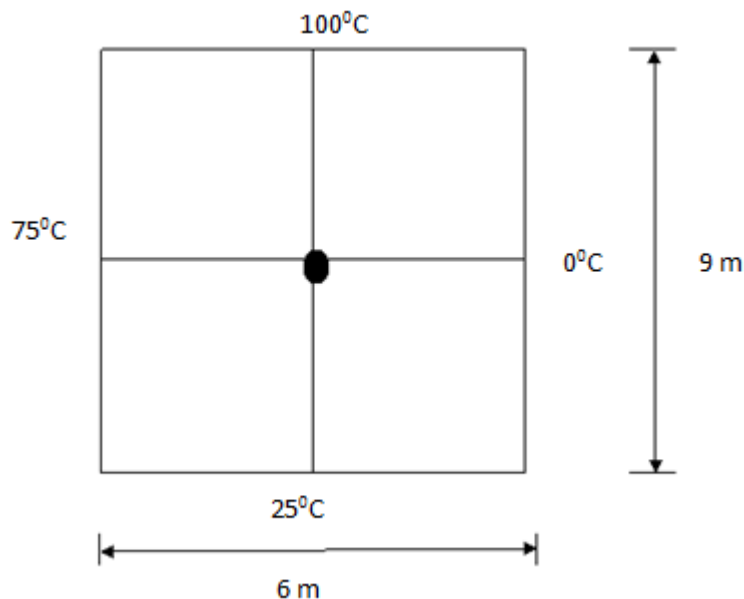
Based on the above data, determine the value of R . [15]

4. Determine approximate value of $\log_e 5$ by performing numerical integration of $\int_0^5 \frac{dx}{4x+5}$. Divide the range into ten equal parts and apply Simpson's one-third rule. [15]
5. The steady state concentration distribution in a one dimensional diffusion process is described by the following second order differential equation:

$$\frac{d^2C}{dx^2} - 2C = 4x^2 - 2x - 4; \text{ At } x = 0: C = 0 \text{ and At } x = 1: \frac{dC}{dx} = -3$$

Using central finite difference method, determine C at $x = 1/3$ and $x = 2/3$. [15]

6. Explain the three types of classification for second order linear partial differential equation giving one example from each category. Find the steady state temperature at the interior node given in the following figure. [6+9]



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Part – II (Open Book)

Maximum Marks - 40

1. Experimental values of volume of a gas at different pressure values are given in the following table.

Gage pressure P (kg/cm ²)	0	1	2	4
Volume V (cm ³)	580	556	520	385

Using Lagrange's interpolation formula, compute the volume of the gas at a gage pressure of 3 kg/cm².

[15]

2. Two dependent variables y and z are functions of one independent variable x and are described by the following pair of ordinary differential equations:

$$\frac{dy}{dx} = x + z \quad \text{and} \quad \frac{dz}{dx} = x - y^2$$

The initial conditions given are: $y(0) = 2$ and $z(0) = 1$

Compute y and z values at $x = 0.1$ using fourth order Runge-Kutta method (Use a step size of 0.1).

[25]