

2006 JAWAHARLAL NEHRU TECHNOLOGICAL UNIVERSITY

IV B.TECH II SEMESTER SUPPLEMENTARY EXAMINATIONS
COMPUTER APPLICATIONS IN CHEMICAL ENGINEERING
(CHEMICAL ENGINEERING)

APR/MAY 2006

TIME - 3 HOUR
MARK - 80**Answer any FIVE Questions**
All Questions carry equal marks

1. Solve by using Runge-Kutta 4th order method: $y' = x^2 + y^2$ with $y(0) = 1$, $h = 0.1$ in the interval $[0, 1]$. [16]
2. Solve by Cramer's rule, the equations: $3x_1 + x_2 - x_3 = 2$, $x_1 + 2x_2 + x_3 = 3$, $-x_1 + x_2 + 4x_3 = 9$. [16]
3. Write a computational procedure to solve the following equation by matrix inversion method $16x + 3y + 3z = 1$, $x + 4y + 3z = 0$, $x + 3y + 4z = 2$. [16]
4. Write a computer program, which uses the Newton-Raphson method for the two equation in two unknowns. [16]
5. For the reaction $\text{CO}_2(\text{g}) + 4\text{H}_2(\text{g}) \rightarrow 2\text{H}_2\text{O}(\text{g}) + \text{CH}_4(\text{g})$ the standard heat of reaction can be expressed as $\Delta H^\circ_T = \Delta H^\circ + \Delta T + (\Delta/2)T^2 + (\Delta/3)T^3$; $\Delta H^\circ = -148345 \text{ J}$; $\Delta = -62.54$; $\Delta = 46.3510 \cdot 10^{-3}$; $\Delta = -7.21 \times 10^{-6}$. Find the relevant temperature at which standard heat of reaction is equal to -183950 J using iterative method. [16]
6. Thermal conductivity of the metal strip was measured at various time intervals during the heating and the values are given in the following table:
- | Time, t (min) | 1 | 2 | 3 | 4 | 5 | 6 |
|-----------------|----|----|-----|-----|-----|-----|
| Temp., T (C) | 70 | 83 | 100 | 124 | 152 | 190 |
- If the relationship between the temperature, T and time, t is of the form $T = \frac{b}{4} + a$ estimate the coefficients (a and b) using least square regression technique and estimate the temperature at $t = 8 \text{ min}$. [16]
7. (a) Illustrate the importance of optimization techniques in chemical engineering giving at least four examples.
- (b) Given the function $f(x) = 80/x + 20x + 20$, find the stationary points and test them for maxima or minima. [8+8]
8. Find the minimum of $y = 10x^2 - 3x + 5$ using Dichotomous search subject to restriction $g(x) = x^2 \leq 10$. Consider 6 calculations only.