

IV B.Tech II Semester Supplementary Examinations, Apr/May 2006
COMPUTER APPLICATIONS IN CHEMICAL ENGINEERING
(Chemical Engineering)

Time: 3 hours

Max Marks: 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 $CO_2(g) + 4H_2(g) \rightarrow 2H_2O(g) + CH_4(g)$ the standard heat of reaction can be expressed as $\Delta H_T^0 = \Delta H' + \Delta\alpha T + (\Delta\beta/2)T^2 + (\Delta\gamma/3)T^3$; $\Delta H' = -148345$ J; $\Delta\alpha = -62.54$; $\Delta\beta = 46.35 \times 10^{-3}$; $\Delta\gamma = -7.21 \times 10^{-6}$. 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 $T = be^{t/4} + a$ estimate the coefficients (a and b) using least square regression technique and estimate the temperature at $t = 8$ 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. [16]
