

IV B.Tech II Semester Supplementary Examinations, April/May 2005
COMPUTER APPLICATIONS IN CHEMICAL ENGINEERING
(Chemical Engineering)

Time: 3 hours

Max Marks: 70

Answer any FIVE Questions
All Questions carry equal marks

1. Solve $dy/dx + xy = 0$ from $x = 0$ to $x = 0.25$ when $y(0) = 1$ by Euler's method.
2. Solve the following equations using Cramer's rule: $x^2z^3/y = e^8$; $y^2z/x = e^4$, $x^3y/z^4 = 1$.
3. Solve the following simultaneous equations. $2.5x_1 + 5.2x_2 = 6.2$; $1.251x_1 + 2.605x_2 = 3.152$ by Gauss Elimination method and correct the answer up to 4 significant digits.
4. a) Solve the equation $e^{-x} - x = 0$ by Newton-Raphson method. b) How does one choose the initial guess value of the root?
5. At 600K the reversible gas-phase reaction $C_2H_4 + Br_2 \leftrightarrow C_2H_4Br_2$ has the rate constants $k_1 = 500$ lit/gmol.hr, $k_2 = 0.032$ hr⁻¹, fractional change in the volume ($\varepsilon_A = -0.7$). Initial molar ratio of Br_2 and C_2H_4 (M) is equal to 2.0. Find the equilibrium conversion using Regular falsi method.
6. An elementary liquid phase reaction $A + B \rightarrow \text{product}$ was carried out in a stirred batch reactor. The variation of concentration w.r.t time is reported in the following table. Fit data using least square regression technique in the second order rate equation and find the rate constant(k). Data: Initial reactant concentration $C_{A0} = 1$ gmol/lit, $C_{B0}/C_{A0} = M = 2$

Time, t (min)	0	5.4	11.7	19.4	28.7	40.5
Concentration (C_A), gmol/lit	1	0.9	0.8	0.7	0.6	0.5

7. Find the minimum and the range of optimum for the function $y = (2x - 90)^2$ using direct search with appropriate step size.
8. Find the minimum of the following function using two point equal interval search method for 6 iterations $f(x) = 10x^2 - 3x$ subject to $-5 < x < 5$
