

IV B.Tech II Semester Regular Examinations, Apr/May 2008
COMPUTER APPLICATION IN CHEMICAL ENGINEERING
 (Chemical Engineering)

Time: 3 hours

Max Marks: 80

Answer any FIVE Questions
 All Questions carry equal marks

1. Using Euler's method, find an approximate value of y corresponding to $x = 1$, given that $dy/dx = x + y$ and $y = 1$ when $x = 0$. [16]
2. Solve the following equations using Cramer's rule: $x+y+z = 6.6$; $x-y+z = 2.2$; $x+2y+3z = 15.2$. [16]
3. Solve by Gauss elimination method $2x + y + z = 10$, $3x + 2y + 3z = 18$, $x + 4y + 9z = 16$. [16]
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? [12+4]
5. Calculate the specific volume of superheated steam at 10Mpa and 623 K(350°C) using the Vander Waals equation: $(p + a/v^2)(v - b) = RT$. Use the Iterative method. Data: $a=0.5531 (m^3)^2.Mpa/(kmol)^2$; $b=0.0304 m^3/kmol$. [16]
6. The steady state substrate (S) for continuous stirred tank fermentor operated at various dilution rates(D) are given below. The fresh feed concentration (S_0) is 700mg/l, calculate the yield factor(Y) and endogenous respiration coefficient(kd) by fitting data using least square regression in the equation of the form: $(S_0 - S)/X = k_d/(Y.D) + 1/Y$ Data: [16]

Dilutino rate (D) h^{-1}	0.3	0.25	0.2	0.12	0.08
Substrate conc.(S)mg/l	45	41	16	8	3.8
Biomass conc.(X) mg/l	326	328	340	342	344

7. Minimize the function $f(x) = x^2 - x$ subject to $-3 < x < 3$ by using Newton's method and quasi Newton's method. Also state the type of function. [16]
8. Find the minimum of the function $y = (2x - 9)^2$
 $0 < x < 10$

using simultaneous search method for 4 experiments. Also find the search effectiveness. [16]

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1. Solve the following differential equation by Runge-Kutta 4th order method: $dy/dx = x^2y^2$ with $y = 1$ at $x = 0$ and $h = 0.1$ in the range $0 \leq x \leq 1$. [16]
2. Solve by Cramer's rule, the equations: $2x_1 - 3x_2 + x_3 = 9$, $x_1 + x_2 + x_3 = 6$, $x_1 - x_2 + x_3 = 2$. [16]
3. Solve the following equation by matrix inversion method $x + 3y + 6z = 2$, $3x - y + 4z = 9$, $x - 4y + 2z = 7$. [16]
4. Develop a program to find the roots of the polynomial equation of order n using Newton-Raphson method. [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. An elementary liquid phase reaction $2A \rightarrow \text{Product}$ is taking place 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 to second order reaction kinetics and find the rate constant (k). Data: Initial reactant concentration $C_{A0} = 1$ gmol/lit. [16]

Time(t),min	0	10	20	30	40	50
Concentration (C_A),gmol/lit	1	0.91	0.83	0.77	0.7	0.64

7. (a) Describe the procedure of identifying extremes for continuous and differentiable functions.
 (b) Determine the convexity of a single variable function $f(Q) = 4Q + 16/Q$ through the evaluation of its first and second derivatives. Also plot the function and its first derivative. [6+10]
8. Minimize the function $f(x) = x^2 - x$ by golden section search for 6 iterations using starting value and step size of x as 3.0 and 0.1 respectively. [16]

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1. Using Euler's method, solve $y' = x + 2y$; $y(0)$ in the range $0 \leq x \leq 1$, with step size $h=0.25$. [16]
2. Solve by Cramer's rule, the equations: $2x_1 - 3x_2 + x_3 = 9$, $x_1 + x_2 + x_3 = 6$, $x_1 - x_2 + x_3 = 2$. [16]
3. Solve the following set of equations by Gauss Elimination method. $x_1 + x_2 + x_3 = 3$; $2x_1 + 3x_2 + x_3 = 6$; $x_1 - x_2 - x_3 = -3$. [16]
4. (a) Solve the simultaneous algebraic equations $X^2 + Y = 3$; $Y^2 + X = 5$ Using regula falsi method.
 (b) Write a computer algorithm for the problem [10+6]
5. A steel pipe of out side diameter 30cm carries steam and its surface temperature is 220°C . It is exposed to surroundings at 25°C . Heat is lost both by convection and radiation. The convective heat transfer coefficient has a value of $22\text{W}/\text{m}^2\text{K}$. If 7.5 cm thickness of the insulating pad with thermal conductivity $36\text{W}/\text{m.K}$ is covered the surface of the steel pipe. Find the surface temperature using regular falsi method. Data: For sphere $Q = (T_2 - T_1) \cdot 2\pi K / \ln(r_1/r_2)$ Heat lost by combined mechanism $= hA(T - T_1) + A\sigma(T^4 - T_1^4)$; $A = \pi D$, $\sigma = 5.67 \times 10^{-8}\text{W}/\text{m}^2\text{K}^4$, K = Thermal conductivity of insulating material, T_1 = Temperature of the surroundings, T_2 = Temperature of the surface of the steel pipe, T = Temperature on the surface of the insulated pipe. [16]
6. The steady state substrate (S) for continuous stirred tank fermentor operated at various dilution rates (D) are given below. The fresh feed concentration (S_0) is $700\text{mg}/\text{l}$, calculate the yield factor (Y) and endogenous respiration coefficient (k_d) by fitting data using least square regression in the equation of the form: $(S_0 - S)/X = k_d/(Y \cdot D) + 1/Y$ Data: [16]

Dilutino rate (D) h^{-1}	0.3	0.25	0.2	0.12	0.08
Substrate conc.(S) mg/l	45	41	16	8	3.8
Biomass conc.(X) mg/l	326	328	340	342	344

7. Find the minimum and the range of optimum for the function
 $y = (2x - 90)^2$
 using direct search with appropriate step size. [16]

8. Find the minimum of the function $y = (2x - 9)^2$

$$0 < x < 10$$

using simultaneous search method for 4 experiments. Also find the search effectiveness. [16]

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1. $dy/dx = y+x$ and $x(0) = 0$. Estimate $x(0.6)$ using $h = 0.2$. [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. Solve the following equation by matrix inversion method $x + 3y + 6z = 2$, $3x - y + 4z = 9$, $x - 4y + 2z = 7$. [16]
4. Given the polynomial equation $X^4 + 0.5X^3 - 8.5X^2 - 0.5X + 7.5 = 0$ Use regula-falsi method to find the roots of the equation to 3 significant digits. [16]
5. The vapour pressure of propane is approximately given by the bamson-Watson equation as follows: $\log P = (-A/T_A) + b - e^{-20(T_r - b)^2}$ where P = vapour pressure in mmHg. T_A = reduced temperature ($T_c = 369.9\text{k}$) $A = 2.6606$, $B = 7.1819$, $b = 0.125$ Calculate the temperature at which propane can exert a vapour pressure of 1000mmHg using Newton-Raphson method. [16]
6. A new microorganism has been discovered which at each cell division yields three daughter cells. The growth rate data during the batch cultivation is given below

Time(t),h	0	.5	1	1.5	2.0
Dry Wt(X),g/l	0.1	0.15	0.23	0.34	0.51

 Fit the above data using least square regression in the exponential growth model $x = a \cdot e^{bt}$ where a and b are constants. [16]
7. (a) Given the function $f(x) = (x^2 + 2)/x$, find the stationary points and test them for maxima and minima.
 (b) Find the root of the following equation by Regula-Falsi method: $x^3 - 2x - 5 = 0$ [8+8]
8. Minimize $y = (2x - 9)^2$
 $0 < x < 10$ for 6 Fibonacci experiments. [16]
