Code No: RR420803 **Set No. 1**

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

Time: 3 hours **Max Marks: 80**

Answer any FIVE Questions
All Questions carry equal marks

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1. Using simple Euler's method solve for y at x = 0.1 from dy/dx = x+y+xy, y(0) = 1, taking step size h = 0.025. [16]

2. In a given electrical network, the equations for the currents i_1, i_2, i_3 are $3i_1+i_2+i_3$= 8; $2i_1 - 3i_2 - 2i_3$ = -5; $7i_1 + 2i_2 - 5i_3 = 0$. Calculate i_1 and i_3 by Cramers rule.[16]

3. Consider the equations. $a_1X + b_1Y + c_1Z = d_1$, $a_2X + b_2Y + c_2Z = d_2$, $a_3X + b_3Y + c_3Z = d_3$. Write a program to solve the above equations using Matrix inversion method. [16]

4. (a) Find the roots of the equation $X^3 - 4X + 1 = 0$ Correct to 3 significant digits using iterative method.
   (b) When does one stop the iterative cycle? [12+4]

5. Calculate the molar volume of methane vapor at 500 K and 10 bar by using the viral equation of the form: PV/RT =1+B/V +C/V^2 where B= -2.19×10^{-4}m^3/mol;C=-1.73×10^{-8}m^6/mol^2. Use the Newton-Raphson method. [16]

6. Fit a curve of the type ae-bx for the data given in the table. [16]

x	0.25	0.5	0.75	1.0	1.25	1.5	1.75	2.00	2.25	2.5
y	3.1	1.7	1.0	0.08	0.42	0.26	0.14	0.09	0.04	0.03

7. (a) Illustrate continuous and discontinuous functions with the shapes of their curves.
   (b) Find the minimum of the expression y = $10x^3 - 4x^2 + 3x - 1$ if -5 ≤ X ≤ 10 by the analytical method. [10+6]

8. (a) Compare the Fibonacci method and modified Fibonacci method by computing the number of experiments required to get an accuracy of $\alpha \leq 0.01$.
   (b) Find the effectiveness of Fibonacci method and modified Fibonacci method when the number of experiments is 10. [8+8]

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Code No: RR420803 **Set No. 2**

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

Time: 3 hours **Max Marks: 80**

Answer any FIVE Questions
All Questions carry equal marks

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1. Use Runge- Kutta 4th order method to approximate y at x = 0.1 and x = 0.2 for dy/dx = x+y with $x_0 = 0$ and $y_0 = 1$ and h = 0.1. [16]

2. Solve by Cramer's rule, the equations:$2x_1+5x_2+3x_3 = 1$,$-x_1+2x_2+x_3=2$,$x_1+x_3+x_2=0$. [16]

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. [16]

4. a) Find the roots of the following polynomial equation using the Newton-Raphson method. $X^4 - 8X^3 + 14.91X^2 + 9.54X - 25.92 = 0$ b) What are the bounds within which the roots lie? [12+4]

5. An elementary liquid phase reaction A + B → R+S is conducted in a multiple reactor system in which 100liters capacity CSTR is used as the first unit and a PFR is used as the second unit. Find the intermediate conversion between the both the units using iterative method. Data: Initial molar ratio of B to A, M =2, Reaction rate constant (k) =0.2 lit/gmol.min, C_{A0}=0.5 gmol/lit and v_0=93.3 lit/min. [16]

6. The specific heat of the Hexane was measured at various temperatures during the heating and given in the following table

Temp(T),K	298	350	400	450	500	550
Cp/R	16.24	18.229	20.07	21.84	23.53	25.14

If the relationship between specific heat and temperature is of the form:
Cp/R=A+BT+CT^2+DT^3.
Estimate the coefficients using polynomial regression. What is the value of specific heat at 700K. [16]

7. (a) Describe the behaviour of different monotonic functions showing the shapes of their curves.
   (b) Given the function f(x) = $1/4x^4 + 2/3x^3 - 5/2x^2$ - 6 x , find the stationary points and test them for maxima and minima. [8+8]

8. Find the minimum of the function
   y = $(2x - 9)^2$
   $0 < x < 10$
   carrying out 4 sequential and equal interval experiments. [16]

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Code No: RR420803 **Set No. 3**

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

Time: 3 hours **Max Marks: 80**

Answer any FIVE Questions
All Questions carry equal marks

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1. Given dy/dx = (y-x)/(y+x) with boundary conditions y = 1 when x = 0, find approximately y for x = 0.1, by Euler's modified method.(5Steps). [16]

2. Solve by Cramer's rule, the equations:$2x_1+3x_2= 12, 4x_1-x_2= 10$. [16]

3. Consider the following sparse set of equations. $2x_1 - 2x_2 = 1; -x_1 + 2x_2 - 3x_3 = -2; -2x_2 + 2x_3 - 4x_4 = -1; x_3 - x - 4 = 3$ Are the zero co-efficients preserved as zeros during Gauss Elimination?. If yes, write a program, which uses the Gauss Elimination method. [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. Given the reactions A + 2B → R ; $r_R = k_1 C_A.C_B^2$ A + B → S ; $r_s = k_2 C_A.C_B, k_2 = 2k_1$ How should the MFR to be operated so as to maximize the desired product R from a single feed consists of $CA_0 = CB_0 = 1.0$.φ(R/A) = $dC_R/-dC_A$, $C_{Rf}=\phi(C_{B0}-C_{Bf})$. Use the Newton raphson method. [16]

6. The thermal conductivity of the metal strip at different temperatures are given in the following table. Fit the data in straight line using least square regression technique. [16]

Temp(T),K	300	320	340	360	380	400
Thermal conductivity(K),W/m.K	7.5	7.9	8.3	8.7	9.1	9.5

7. (a) Explain the necessary and sufficient conditions for the extreme of an unconstrained function.
   (b) Determine the nature of stationary point of the function f(x) = -3x^5 + 10x^3 - 20

   [8+8]

8. Find the minimum of y = 10x^2− 3x + 5 using Dichotomous search subject to restriction g(x) = x^2 5 ≤ 10. Consider 6 calculations only. [16]

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Code No: RR420803 **Set No. 4**

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COMPUTER APPLICATION IN CHEMICAL ENGINEERING
(Chemical Engineering)

Time: 3 hours **Max Marks: 80**

Answer any FIVE Questions
All Questions carry equal marks

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1. Apply Runge-Kutta 2nd order method to find an approximate value of y when x =0.2 given that dy/dx = x+y and y = 1 when x = 0. [16]

2. Solve the following equations using Cramer's rule: $x^2z^3/y = e^8$; $y^2z/x = e^4$, $x^3y/z^4 = 1$. [16]

3. In a given electrical network, the equations for the currents i_1, i_2, i_3 are $3i_1 + i_2 + i_3$ = 8 ; $2i_1 - 3i_2 - 2i_3$ = -5; $7i_1 + 2i_2 - 5i_3 = 0$ by Matrix inversion method. [16]

4. Develop a computer program which uses the Newton-Raphson method to calculate the specific volume of a pure gas at a given temperature and pressure by using the Beattie-Bridgeman equation of state PV = RT $+\beta/\mathrm{V}+\gamma/\mathrm{V}^2+\delta/\mathrm{V}^3$.The variable β,$\gamma$andδ are empirical functions of temperature β = RT B_0 - A_0- RC/T^2 γ = - RTB_0b $+\alpha\mathrm{A}_0-\mathrm{RB}_0\mathrm{C}/\mathrm{T}^2$ δ= $\mathrm{RB}_0\mathrm{bC}/\mathrm{T}^2$ Where constants $\mathrm{A}_0, \mathrm{B}_0, \alpha, \mathrm{b}, \mathrm{C}$ are given. [16]

5. The friction factor for the flow of a fluid through a pipe is a function of Reynolds number, Re. When the flow is turbulent for Re 4200, the friction factor is also a function of roughness factor e/D of the pipe and may he estimated from the relation. $\frac{1}{\sqrt{f}=3.48-4\log}\left[2\frac{e}{D}+\frac{9.35}{\mathrm{R}e\sqrt{f}}\right]$ Calculate the value of f at Re = 20,000 and e/D = 0.005 using iterative method. [16]

6. Find the overall order of the irreversible reaction $2H_2$ +2NO $\rightarrow N_2 + 2H_2O$ from the following constant volume data using equimolar amounts of hydrogen and nitric acid. Use the least square regression technique. Data: [16]

Total pressure ($\pi_\circ$),mm Hg	200	240	280	320	360
Half-life($t_{1/2}$),sec	265	186	115	104	67

7. Find the minimum of the function
   y = $(2x - 9)^2$
   adopting direct search with accelerating step size. [16]

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 [16]

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