Code No: NR420803 **Set No.1**

**IV B.Tech. II Semester Supplementary Examinations, July -2005**
**COMPUTER APPLICATIONS 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. Solve the following differential equation by Runge-Kutta 4$^{th}$ order method: dy/dx = $x^2y^2$ xy with y = 1 at x = 0 and h = 0.1 in the range $0 \leq x \leq 1$ .

2. Solve the following equations using Cramer's rule: x+3y+6z = 2; 3 x-y+4z = 9; x-4y+2z = 7.

3. Solve the following equation by matrix inversion method x + y + 2z = 4 , 2x - y + 3z = 9 , 3x - y - z = 2

4. Determine the two smallest roots of the following equation F (x) = xcosx + cosx = 0 and correct to 3 significant digits using false position method.

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 $\Delta H^0_T$ =$\Delta$H' + $\Delta\alpha$T + $(\Delta\beta/2)T^2 + (\Delta\gamma/3)T^3$ ; $\Delta$H'=-148345 j; $\Delta\alpha$=-62.54; $\Delta\beta$=$46.3510^{-3}$ ; $\Delta\gamma = -7.21 \times 10^{-6}$ . Find the relevant temperature at which standard heat of reaction is equal to -183950j using iterative method.

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+C$T^2$+D$T^3$ Estimate the coefficients using polynomial regression. What is the value of specific heat at 700K.

7. a) Describe the Newton-Raphson method of solving a single variable function.

   b) Find the root of the following equation by Newton-Raphson method. $x^3 - 5x^2$ + 4 x - 3 = 0

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.

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Code No: NR420803 **Set No.2**

**IV B.Tech. II Semester Supplementary Examinations, July -2005**
**COMPUTER APPLICATIONS 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. Solve the differential equation : dy/dx = -$x^2$+$y^2$ , y = 2 at x = 0, by modified Euler's method and obtain y at x =0.2 in two stages of 0.1 each.

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

3. Solve the following equation by matrix inversion method 2x + 3y + 2 = 9, x + 2y + 3z = 6, 3x + y + 2z = 8.

4. Find the three roots of the equation $x^3 - 4x + 1 = 0$ to 3 significant digits using Newton-Raphson method.

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 $\Delta H^0_T$ =ΔH' + ΔαT + $(\Delta\beta/2)T^2 + (\Delta\gamma/3)T^3$ ; ΔH'=-148345 j; Δα=-62.54; $\Delta\beta$=46.3510$^{-3}$ ; $\Delta\gamma = -7.21 \times 10^{-6}$ . Find the relevant temperature at which standard heat of reaction is equal to -183950j using iterative method.

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.e$^{bt}$ where a and b are constants.

7. a) Describe the Newton-Raphson method of solving a single variable function.

   b) Find the root of the following equation by Newton-Raphson method. $x^3 - 5x^2$ + 4 x - 3 = 0

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.

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Code No: NR420803 **Set No.3**

**IV B.Tech. II Semester Supplementary Examinations, July -2005**
**COMPUTER APPLICATIONS 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. Give the algorithm for the solution of differential equation of the form dy/dx = f(x,y) using Euler's method.

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

3. Solve by Gauss elimination method 2x + y + z = 10 ,3x + 2y + 3z = 18, x + 4y + 9z = 16.

4. Find the negative root of the equation $x^3 - 21x + 3500 = 0$ correct to 2 decimal places by Newton-raphson method and also develop a computer algorithm.

5. Ethane gas is processed at 7.3 Mpa a and 423 K(150°C ) if following Beattie- Bridgeman equation of state P = $[RT(1-\varepsilon)/v^2](v + B) - A/v^2$ where A=$A_0$(1 a/v); B=$B_0$(1 b/v); $\varepsilon$= C/v$T^3$ Data: For ethane: $A_0$= 0.588 Mpa$(m^3)^2/(kmol)^2$, $B_0$=0.094 $m^3$/kmol, a=0.05861 $m^3$/kmol, b=0.01915 $m^3$/kmol and C = $90 \times 10^4$ $m^3(K)^2$/kmol. Find the molar volume of the ethane gas at the conditions using iterative method.

6. During the protein estimation by the Lowrys method using spectrophotometer the following data were obtained

| mg of protein(X) | 0 | 1 | 3 | 4 | 6 | 8 | 9 | 11 |
|---|---|---|---|---|---|---|---|---|
| Absorbancy (y) | 0 | 0.1 | 0.2 | 0.4 | 0.5 | 0.6 | 0.7 | 0.8 |

   Use the least square regression to fit a straight line to the above data.

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. a) Determine the number of experiments required to locate the final region with in 1 % of the original search region by Fibonacci and preplanned regular intervals search methods.

   b) Find the effectiveness of Fibinacci and preplanned regular intervals methods when the number of experiments is 6.

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Code No: NR420803 **Set No.4**

**IV B.Tech. II Semester Supplementary Examinations, July -2005**
**COMPUTER APPLICATIONS 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. Solve by using Runge-Kutta $4^{th}$ order method :dy/dx = (1-x)$y^2$ with y(0) = 1.5 , h = 0.1 for $0 \leq x \leq 0.5$.

2. Solve the following equations using Cramer's rule: x+y+z = 3; x+2y+3z = 4; x+4y+9z = 6.

3. Write a computational procedure and to solve the following equation by matrix inversion method 2x - 3y + z = -1, x + 4y + 5z = 25, 3x - 4y + z = 2.

4. a) Find the roots of $X^2 - 25 = 0$ numerically using Regula-falsi method. b) Write the computational procedure to evaluate the roots of the equation.

5. Hydrolysis of rice bran oil was conducted using immobilized lipase enzyme in a packed bed reactor. Due to the formation of external film around the immobilized solid particle, substrate diffuses through the film to the solid surface and then getting reacted. The rate of transfer of substrate through the film can be expressed as $K_{la}(S_0-S)$ . The rate of reaction at the solid surface can be expressed using Michaelis-Menten kinetics $V = V_{max}.S/(k_m+s)$ . Find the substrate concentration at the solid-liquid interface, when the rate of transfer of substrate balances the reaction rate. Use the Iterative method. Data: Mass transfer coefficient ($K_{La}$) = $0.08min^{-1}$ , Apparent Michaelis constants,$V_{max}$= 0.02 gmol/lit.min, $K_m$=0.2gmol/lit and Initial substrate concentration ($S_0$)=0.4 gmol/lit

6. For the following data for y measured for a set of values of x plot y vs x. From the plot guess the nature of the curve to be fitted. Using least squares method fit the curve.

| x | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 |
|---|---|---|---|---|---|---|---|---|---|
| y | 7.6 | 13.2 | 27.4 | 33.0 | 62.5 | 86.4 | 115.1 | 147.0 | 182.2 |

7. a) Give mathematical definitions and show the shape of curves for convex, concave and convex-concave functions.

   b) Express mathematically which of these functions are convex, concave and convex-concave : (i) f(x) = $2x^2$ (ii) f(x) = - $2x^2$ (iii) f(x) = $x^3 - 3x^2$

8. Minimize y = $(2x - 9)^2$

   $0 < x < 10$ for 6 Fibonacci experiments.

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