S.E - III Sem - Chem.

Computer Programming & Numerical Methods

(4)

SE/III/eBGS/CHEM/CP&NM

QP Code : 30669

(3 Hours) **[Total Marks : 80**

N.B. : 1) Question No.1 is compulsory

2) Answer any three questions from remaining questions

3) Assume data if necessary and specify assumptions clearly

Q.1 a) Solve following system of equations by using Gauss-Elimination Method 5 marks

$x+y+z=7 \quad x+2y+3z=16 \quad x+3y+4z=22$

b) Use Crank-Nicholson Scheme to solve, $u_{xx}=u_t, 0<x<1,\ t>0$, $h=\frac{1}{4}$, $k=\frac{1}{8}$ 5 marks

Given $u(x,0)=0$, $u(0,t)=0$, $u(1,t)=50t$ Compute u for 1-step in t-direction

c) Explain the use of 'if-else ' in SciLab with appropriate example 5 marks

d) A chemical reaction is carried out in a batch of reactor and the change in concentration of 5 marks

reactant is given by $\frac{dC_A}{dt}=\frac{C_A}{0.6+2C_A}$, initially at $t=0$, $C_A=1$. Find C_A at $t=1$ by using

Runge Kutta Method of second order with $h=0.5$

Q.2 a) Use Bender Schmidt Method to solve, $\frac{\partial^2 u}{\partial x^2}=\frac{1}{4}\frac{\partial u}{\partial t}$ given $u(0,t)=0=u(8,t)$, 10 marks

$u(x,0)=4x-\frac{x^2}{2}$ Find u in the range taking $h=1$ upto $t=1$

b) Find the root of the equation $3x-\sqrt{1+\sin x}=0$ upto four decimal places using Bisection Method 10 marks

Q.3 a) Use Regula Falsi Method to find the root of the equation $x\log_{10}x=2$ upto three decimal places 7 marks

b) Discuss the convergence of Newton Raphson Method 6 marks

[TURN OVER

c) Solve $\frac{\partial^2 p}{\partial x^2}+\frac{\partial^2 p}{\partial y^2}=0$, if $p(0,y)=0$, $p(x,0)=0$, $p(4,y)=y$, $p(x,4)=x$ 7 m

where $0 \le x \le 4$, $0 \le y \le 4$ by draw the mesh for given data

Q4 In a particular reaction equilibrium problem the following equations are obtained 20 m

$$C_A = 40-20x_1-10x_2 \quad C_B = 10-10x_2 \quad C_C = 20x_1-30x_2 \quad C_D = 15-5x_1$$

And the equilibrium position is calculated by the equations

$$f_1 = \frac{C_C}{C_A C_D}-6\times10^{-4}=0 \qquad f_2 = \frac{C_C}{C_A^{\,2} C_B}-5\times10^{-2}=0$$

Use appropriate numerical method to calculate the equilibrium position

Q.5 a) Lee and Duffy relate the friction factor of flow of suspension of fibrous particles to the 10 m

Reynolds Number by the expression $\frac{1}{\sqrt{f}}=\left(\frac{1}{k}\right)\ln\left(\mathrm{Re}\sqrt{f}\right)+\left(14-\frac{5.6}{k}\right)$

For the suspension with 0.08% concentration, k=0.28. What is the value of f when $\mathrm{Re}=3750$

Use the Iterative Method to find the friction factor correct upto four decimal places

b) Solve the following system of equation by Gauss- Jordan Method and LU-Decomposition 10 m

$x+y+z=3 \qquad x+4y+9z=6 \qquad x+2y+3z=4$

Q.6 a) Calculate the volume of superheated steam at $100atm$ and $350^\circ C$ using the equation 10 m

$\left(P+\frac{a}{v^2}\right)(v-b)=RT$, Newton-Raphson Method, for initial value of v use Ideal gas equation

where $a=\frac{27R^2T_c^{\,2}}{64P_c}$, $b=\frac{RT_c}{8P_c}$, $Tc=647.11Kelvin$, $Pc=220.76atm$

b) Solve $\frac{dy}{dx}=x^2(1+y)$, $y(1)=1$, $h=0.1$. Find the value of $y(1.4)_P$ and $y(1.4)_C$ by Adam Bashforth 10 m