S.E - III Sem - Chem.

Computer Programming & Numerical Methods. 3/12/15

(1)

SE/III/CBGS/CHEM/CP&NM

**QP Code : 5177**

(REVISED COURSE)

(3 Hours) (28) [Total Marks: 80

N.B. :

1) Question – 1 is compulsory. Answer any three questions from remaining.

2) Assume data if necessary and specify the assumptions clearly

3) Draw neat sketches wherever required.

4) Answer to the sub-questions of an individual question should be grouped and written together i.e. one below the other.

1\. (a) Explain how to use 'for' loop in SciLab with appropriate example. [05]

(b) Use Crank-Nicholson Scheme to solve, [05]

$$u_{xx} = u_t \quad 0 \le x \le 1 \quad t > 0 \quad h = \frac{1}{4} \quad k = \frac{1}{4}$$

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

(c) Show progress of bisection method using graphical representation. [05]

(d) Solve following system of equations, [05]

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

2\. Liquid Molar volume of n-butane at 350 K and 9.4573 bar may be calculated using Redlich-Kwong equation as given below, [20]

$$V^l = \frac{zRT}{p}$$

where,

$$z = \beta + z(z+\beta)\left(\frac{1+\beta-z}{q\beta}\right)$$

$$\beta = 0.08664\frac{p_r}{T_r} \quad p_r = \frac{p}{p_c} \quad T_r = \frac{T}{T_c} \quad q = 6.6048$$

for n-butane, $T_c = 425.1$K, $p_c = 37.96$bar.
Calculate liquid molar volume for n-butane at given condition using Newton-Raphson method starting with $z = \beta$.

3\. (a) Solve following set of equations using Gauss-Seidel and Gauss-Jordan Method [14]

$$2x_1 - 3x_2 + x_3 = -11$$
$$3x_1 + 4x_2 - 3x_3 = -34$$
$$x_1 + 5x_2 - 2x_3 = -17$$

(b) Write Laplace equation and express it in difference form using Taylor's series expansion. [06]

4. A chemical reactor that has a single second order reaction and a outlet flowrate that is a linear function of height has the following model: [20]

$$\frac{dVC}{dt} = F_{in}C_{in} - FC - kVC^2$$
$$\frac{dV}{dt} = F_{in} - F$$

where, $F = \beta V$.
The parameters and variables are as given below.

$F_{in}$ = inlet flowrate, (2 LPM)
$C_{in}$ = inlet concentration, (1 gmol/lit)
$k$ = reaction rate constant, (2 lit/(gmol-min))
$\beta = 1\ \text{min}^{-1}$
$V$ = reaction mixture volume, (at t = 0, 1 lit)
$C$ = concentration in reactor, (at t = 0, 0.5 gmol/lit)

Find the concentration and volume after one minute using Runge-Kutta second order method.

5. (a) Friction factor in commercial pipe for turbulent flow can be calculated using Colebrook equation. If roughness factor(k) for carbon steel pipe is 0.00015 m for a pipe with ID (D) 0.315 m, using suitable numerical method calculate friction factor (f) if Reynolds number(Re) is 125,000. [12]
Colebrook equation,

$$\frac{1}{\sqrt{f}} = -2.0 \log\left(\frac{k/D}{3.7} + \frac{2.51}{Re\sqrt{f}}\right)$$

(b) Find the root of the function $f(x) = \frac{3x^2}{16} - \frac{27}{4}$ using Regula-Falci method. Consider the span [0,10]. [08]

6. (a) Solve the following system by Gaussian Elimination with and without partial pivoting and comment on the results: [10]

$$\begin{bmatrix} 2 & 1 & 1 & -2 \\ 4 & 0 & 2 & 1 \\ 3 & 2 & 2 & 0 \\ 1 & 3 & 2 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 0 \\ 8 \\ 7 \\ 3 \end{bmatrix}$$

(b) Solve the following system by LU decomposition: [10]

$$A = \begin{bmatrix} 4 & 0 & -1 & 3 \\ 2 & 1 & -2 & 0 \\ 0 & 3 & 2 & -2 \\ 1 & 1 & 0 & 5 \end{bmatrix} \qquad b_1 = \begin{bmatrix} 0 \\ 1 \\ 4 \\ -2 \end{bmatrix}$$

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