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UNIVERSITY OF PETROLEUM AND ENERGY STUDIES

End Semester Examination – December 2017

Program/course: M. Tech Chemical Engineering (PD)

Semester – I

Subject: Chemical Engineering Computing

Max. Marks : 100

Code : CHPD7002

Duration : 3 Hrs

No. of page/s: 04

*The question paper consists of three sections. Answer the questions section wise in the answer booklet.

- Note:** 1) Attempt *all* the questions.
2) Assume suitable data wherever necessary. The notations used here have the usual meanings.

SECTION – A (Total Marks: 2 x 10 = 20)

Q.1 Obtain the eigenvalues and eigenvectors for the symmetric matrix

$$\begin{bmatrix} 3 & 1 \\ 1 & 3/2 \end{bmatrix}$$

Use $x_2 = 1$ as an additional condition. Check if the eigenvalues are real for this case and if the eigenvectors are orthogonal. [10]

Q.2 Consider the following set of coupled ODE-IVPs:

$$\frac{dy_1}{dt} = -0.2y_1 + 0.2y_2 = f_1(t, y); y_1(0) = 0$$

$$\frac{dy_2}{dt} = 10y_1 - (60 + 0.125t)y_2 + 0.124t = f_2(t, y); y_2(0) = 0$$

- (a) Obtain the appropriate eigenvalues at $t = 0, 1, 5$ and 10 analytically
(b) State whether the ODEs are stable and suggest the largest value of h for which stable solutions are expected using the 4th order explicit RK technique. [10]

SECTION – B (Total Marks: 4 x 15 = 60)

Q.3 Consider a separation system as shown in Fig. 1. By setting up the mass balances, calculate the mass flow rates of each outlet streams (x_1 , x_2 and x_3) using Gauss elimination with backward sweep. [15]

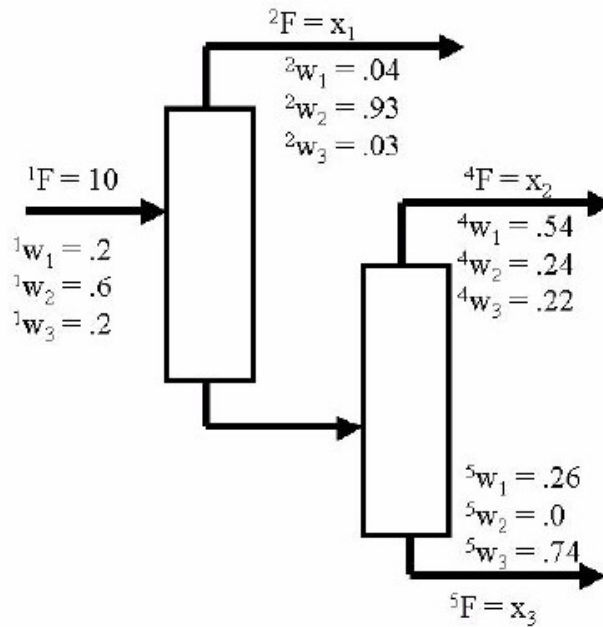


Fig. 1: A Separation system

Q.4 Consider the following non-linear ODE-BVP

$$\frac{d^2y}{dx^2} + 5\frac{dy}{dx} - 3y^3 = 0$$

$$x = 0: \frac{dy}{dx} = 0; \quad x = 1: y(x = 1) = 3$$

Using the OC for the non-symmetric case, and with $N + 2 = 4$:

- (a) What are the numerical values of x_2 and x_3 [03]
- (b) Give the simplified OC equation for $x_1 = 0$ (take ALL the constants and the non-linear terms to the right hand side) [04]



- (c) Give the simplified OC equation for point 2 and 3 (keep B_{ij} and A_{ij} terms separate)
[08]

Q.5 (a) Solve using the Newton-Raphson technique:

$$y = 1 + 2(1.2 - y)^2 \exp \left[10 \left(1 - \frac{1}{y} \right) \right]$$

Use $y^{(1)} = 1.05$. Obtain $y^{(2)}$ and $y^{(3)}$. **[12]**

(b) Explain in brief about the condition for convergence for successive substitutions. **[03]**

Q.6 The desorption of a gas from a liquid stream in a wetted-wall column can be described by the following PDE:

$$(1 - \eta^2) \frac{f}{\eta} = \frac{\partial^2 f}{\eta^2}$$

$$\frac{f}{\eta} = 0 \text{ at } \eta = 1$$

$$f = 0 \text{ at } \eta = 0$$

$$f = 1 \text{ at } t = 0$$

Note that the problem as defined above is not symmetric about $\eta=0$. Carry out an orthogonal collocation solution in the η direction, using $N = 2$ (i.e. two internal OC points) and simplify to obtain a set of two ODE-IVPs. Do not solve these. **[15]**

SECTION – C (Total Marks: 1 x 20 = 20)

Q.7 The concentration of salt x in a homemade soap maker is given as a function of time by

$$\frac{dx}{dt} = 37.5 - 3.5x$$

At the initial time, $t=0$, the salt concentration in the tank is 50 g/L. Using Runge-Kutta 4th order method and a step size of, $h=1.5 \text{ min}$, what is the salt concentration after 3

minutes?

The exact solution of the ordinary differential equation is given by

$$x(t) = 10.714 + 39.286 e^{-3.5t}$$

Compare the exact solution with the numerical solution and comment on the result. [20]

Data:

TABLE 6.1
Matrices for the Orthogonal Collocation Technique [5] (non-symmetric)*
[0 ≤ x ≤ 1, W(x) = 1 in Eq. 6.19]

N+2	x	w	A	B
3	$\begin{pmatrix} 0 \\ 0.5 \\ 1 \end{pmatrix}$	$\begin{pmatrix} \frac{1}{6} \\ \frac{2}{3} \\ \frac{1}{6} \end{pmatrix}$	$\begin{pmatrix} -3 & 4 & -1 \\ -1 & 0 & 1 \\ 1 & -4 & 3 \end{pmatrix}$	$\begin{pmatrix} 4 & -8 & 4 \\ 4 & -8 & 4 \\ 4 & -8 & 4 \end{pmatrix}$
4	$\begin{pmatrix} 0 \\ 0.21132 \\ 0.78868 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix}$	$\begin{pmatrix} -7 & 8.196 & -2.196 & 1 \\ -2.732 & 1.732 & 1.732 & -0.7321 \\ 0.7321 & -1.732 & -1.732 & 2.732 \\ -1 & 2.196 & -8.196 & 7 \end{pmatrix}$	$\begin{pmatrix} 24 & -37.18 & 25.18 & -12 \\ 16.39 & -24 & 12 & -4.392 \\ -4.392 & 12 & -24 & 16.39 \\ -12 & 25.18 & -37.18 & 24 \end{pmatrix}$
5	$\begin{pmatrix} 0 \\ 0.11270 \\ 0.50000 \\ 0.88730 \\ 1 \end{pmatrix}$	$\begin{pmatrix} 0 \\ 0.27778 \\ 0.44444 \\ 0.27778 \\ 0 \end{pmatrix}$	use program in Ref. 12 to generate these	

compiled from Ref. 5)
given by Eq. 6.23

[Ref: Numerical Methods for Engineers, Gupta S. K., 3rd Edition, New Age International]