Name : ....

Roll No. : ....

Invigilator's Signature : ....

CS/M.Tech (CHE)/SEM-1/CHE-04/2010-11

2010-11

ADVANCE NUMERICAL METHODS IN CHEMICAL ENGINEERING

Time Allotted : 3 Hours | Full Marks : 70

The figures in the margin indicate full marks.

Candidates are required to give their answers in their own words as far as practicable.

Answer any *five* questions. $5 \times 14 = 70$

1. a) Find the eigenvalues and eigenvectors of the matrix

$$A = \begin{pmatrix} 3 & 1 & -1 \\ 2 & 2 & -1 \\ 2 & 2 & 0 \end{pmatrix}$$

b) Find for what values of K, the following equations $x + y + z = 1$, $2x + y + 4z = K$ and $4x + y + 10z = K^2$ have solutions and solve them completely in each case.

2. a) Certain corresponding values of x and $\log_{10} x$ are (300, 2·4771), (304, 2·4829), (305, 2·4843) and (307, 2·4871). Find $\log_{10} 301$ using Lagrange's interpolation formula.

b) Given $\frac{dy}{dx} = y - x$, where $x_0 = 0$, $y_0 = 2$ with $h = 0·2$. Determine y (0·2) correct to four decimal places by Runge-Kutta method. Find the analytical solution and find the error.

3. a) Construct using Gram-Schmidt process an orthogonal basis of $V_3(R)$, given a basis $X_1 = [1,\ 1,\ 1]'$, $X_2 = [1,\ -2,\ 1]'$, $X_3 = [1,\ 2,\ 3]'$.

   b) Given the vectors $X_1 = [1,\ 2,\ 3]'$ and $X_2 = [2,\ -3,\ 4]'$, find

      i) their inner product

      ii) the length of each.

4. a) What is stiff-differential equation ? Solve the differential equation $\frac{dy}{dx} = -100y + 99e^{-x}$ with y (0) = 0 to justify the definition.

   b) Develop the Gear formula

   $\nabla y_{n+1} + \frac{1}{2}\nabla^2 y_{n+1} + \frac{1}{3}\nabla^3 y_{n+1} = hy'_{n+1}$ where ∇ is the backward difference operator. Show that it is equivalent to $\nabla y_{n+1} = \frac{18}{11} y_n - \frac{9}{11} y_{n-1} + \frac{2}{11} y_{n-2} + \frac{6}{11} hy'_{n+1}$ and $y'_{n+1} = f(x_{n+1},\ y_{n+1})$.

5. Apply Galerkin's method to solve the boundary value problem (BVP) $y'' + y + x = 0,\ y(0) = y(1) = 0$.

6. Solve the BVP $y'' = -x^2,\ y(0) = y(1) = 0$ by finite element method.

7. Construct a set of polynomials $P_{m,\,N}\ (t)$ of degree m = 0, 1, 2 ...... such that $P_{m,\,n}\ (t)$. $P_{m,\,N}\ (t)$ = 0 for $m > n$, so that the polynomials are orthogonal over the set of arguments t.

8. Determine the coefficients a_k so that

   $p(x) = a_0 P_{0,\,N} + (t) + a_1 P_{1,\,N}\ (t) + ... + a_m P_{m,\,N}\ (t)$ with

   $t = (x - x_0)/h$, will be the least squares polynomial of degree m for the data $(x_i,\ y_i)$ t = 0, 1, 2, ... N.

9. Find the standard five-point formula of the finite difference analogue of Laplace's equation $u_{xx} + u_{yy} = 0$.

10. Use Gram-Schmidt orthogonalisation process to find the first two orthogonal polynomials on [–1, 1] with respect to the weight function w (x) = 1.