NUMERICAL METHODS IN CHEMICAL ENGINEERING
(CHEN 2202)

Time Allotted : 2½ hrs **Full Marks : 60**

Figures out of the right margin indicate full marks.

Candidates are required to answer Group A and any 4 (four) from Group B to E, taking one from each group.

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

1. Answer any twelve: **12 × 1 = 12**

Choose the correct alternative for the following

(i) The order of truncation error in central difference scheme is _____, where 'h' is the step size.
(a) O(h) (b) $O(h^2)$ (c) O(1/h) (d) $O(1/h^2)$

(ii) In quadratic interpolation with 'n' number of data points, the number of equations required to get the constants solved for every spline is equal to _____
(a) n (b) 2n (c) 3n (d) 4n

(iii) The convergence criterion for an equation f(x)=0 during finding of the root using Newton-Raphson method is given by _____, where ξ is any intermediate point between two iterations x_i and x_{i+1}, and α is the root of the equation.
(a) $\frac{e^{i+1}}{e^i}=\left|\frac{f''(\xi)}{2f'(\alpha)}\right|$ (b) $\frac{e^{i+1}}{(e^i)^2}=\left|\frac{f''(\xi)}{2f'(\alpha)}\right|$ (c) $\frac{e^{i+1}}{e^i}=\left|\frac{f'(\xi)}{2f''(\alpha)}\right|$ (d) $\frac{e^{i+1}}{(e^i)^2}=\left|\frac{f'(\xi)}{2f''(\alpha)}\right|$

(iv) The condition number for a function $f(x)=\sqrt{x+1}-\sqrt{x}$ is _____
(a) more than 1
(b) in between 0.5 and 1
(c) less than 0.5
(d) oscillatory within 0.5 and 1

(v) The matrix $A=\begin{bmatrix}1 & 1\\ 1 & 1/2\end{bmatrix}$ is _____
(a) positive definite
(b) negative definite
(c) positive semi-definite
(d) negative semi-definite

(vi) In order to solve 1st order simultaneous set of equations the condition to apply Gauss-Siedel iterative method_____.
(a) is the determinant of the coefficient matrix is not equal to zero
(b) the diagonal elements must not be equal to zero
(c) the matrix must be diagonally dominant
(d) all of these

(vii) The equation given by $\frac{d^2T}{dx^2}-K(T-T_s)=0$ which is a mathematical model for heat transfer along the length of a rod and will require _____ boundary conditions
(a) 1 (b) 0 (c) 2 (d) 4

(viii) The series reaction $A \rightarrow B \rightarrow C$ takes place in a mixed reactor. The time varying concentration of *A, B* and *C* are required. The mathematical model of the system will give rise to
(a) two first order ODE
(b) three algebraic equation
(c) three first order ODE
(d) two second order ODE

(ix) During unsteady state heat conduction process condition for obtaining a stable iterative solution through explicit method can be possible with all the positive coefficients is _____, where α is the thermal diffusivity.
(a) $\Delta t<\frac{1}{2\alpha}(\Delta x)$ (b) $\Delta t<\frac{1}{2\alpha}(\Delta x)^2$ (c) $\Delta t<\frac{\alpha}{2}(\Delta x)^2$ (d) $\Delta t<\frac{\alpha}{2}(\Delta x)$

(x) If _____, then f(x,y) has a saddle point, where 'H' is the Hessian.
(a) |H|>0 (b) |H|<0 and $\frac{\partial^2 f}{\partial x^2}<0$ (c) |H|<0 (d) |H|>0 and $\frac{\partial^2 f}{\partial x^2}>0$

Fill in the blanks with the correct word

(xi) The mathematical error during interpolation of a polynomial $f(x)=-2+3(x-1)-4(x-1)(x-4)$ at x=2 is equal to_____.

(xii) In the interval [1 8] the area under the curve of a function $f(x)=4x^2+3$ using SIMPSON's rule is equal to _____, when h =4.

(xiii) Spectral radius for a matrix $A=\begin{bmatrix}3 & 0\\ 0 & 2\end{bmatrix}$ is equal to _____.

(xiv) The ODE :$\frac{dy}{dt}=\frac{t^2}{y}$ $where\ y(0)=1$can be solved with the Euler Explict method using a time step of 0.1. At *t = 0.1*, the absolute error between the analytical and numerical solution is _____

(xv) For the equation, $\frac{dn}{dt}=-0.8\,n^{1.5}+(1-e^{-3t})\ where\ n(0)=1000$ .Using the Euler Implicit method forthe marching equation n_{i+1}= _____.

Group - B

2. (a) What are the differences between true error and approximate error? *[(CO1)(Understand/LOCQ)]*

(b) Calculate fl(f(100000)) with six digits chopping from a function $f(x)=x\left(\sqrt{x+1}-\sqrt{x}\right)$. *[(CO1)(Apply/IOCQ)]*

(c) To find how much heat is required to bring a kettle of water to its boiling point you are asked to calculate specific heat at 61°C. Calculate it at 61°C using Lagrangian interpolation technique from the following information. *[(CO2)(Apply/IOCQ)]*

T (oC)	42	52	82
Specific heat (J/kgK)	4179	4186	4199

2 + 6 + 4 = 12

3. (a) Calculate the bubble point for acetone-water system at 101.325 kPa and feed composition of 50mole % each using Newton-Raphson method. Show three iterations.

$$P=\sum_{i=1}^{2}x_iP_i^{sat};1:\text{Acetone},2:\text{Water}$$

$$\ln P_1^{sat}=4.42-\frac{1312.25}{T-32.45}$$

$$\ln P_2^{sat}=3.56-\frac{643.75}{T-198.04}$$

[(CO2)(Analyse/HOCQ)]

(b) Show that if a function f(x)=x-g(x) is solved iteratively such that $x_{i+1}=g(x_i)$, the convergence criteria becomes satisfied when $|g'(\xi)|<1$, where $x_{i+1}<\xi<x_i$. *[(CO2)(Apply/LOCQ)]*

(c) Show that the truncation error order will be of $O(h^2)$ in case of central difference scheme, where $h=x_{i+1}-x_i$. *[(CO2)(Understand/LOCQ)]*

7 + 2 + 3 = 12

Group - C

4. (a) Consider a steady state heat transfer at constant wall temperature in the fully developed region of a tubular laminar parabolic flow (Fig. 1), where the velocity profile is given as $u=2u_0\left(1-\frac{r^2}{R^2}\right)$. The dimensionless steady state temperature θ(z,r) in the fluid is analytically derived and given as $\theta(z,r)=-4z-r^2+\frac{r^4}{4}+\frac{7}{24}$. The mixing cup temperature is given as

$$\theta_{mix}=\frac{\int_0^1\theta(z,r)\left(1-r^2\right)rdr}{\int_0^1\left(1-r^2\right)rdr}$$

Determine the mixing cup temperature at z=0.5 using Simpson's 1/3rd rule. Consider Δr=0.25.

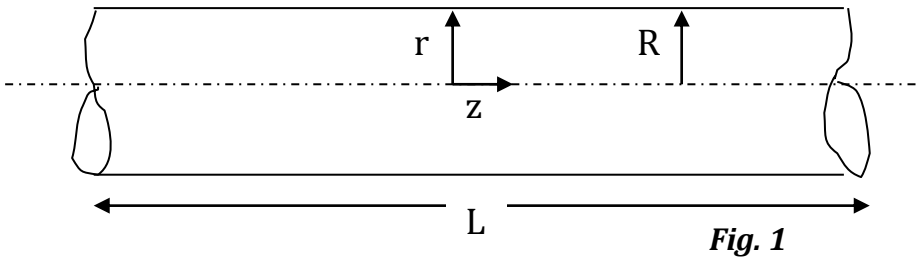

Fig. 1

[(CO4)(Analyse/HOCQ)]

(b) Show that during integration with the trapezoidal rule the order of the error on one segment is $O(h^3)$, where 'h' is the length of the segment. *[(CO4)(Remember/LOCQ)]*

8 + 4 = 12

5. (a) Fig. 2 shows a chemical process consists of 3 reactors (R1, R2 and R3) linked by pipes. The mass flow rate of a chemical (gps) through each pipe is equal to its concentration in each reactor, c (g/m^3) multiplied by the volume flow rate (m^3/s) of the pipe. Assume the system is at a steady state, so that the transfer into each reactor will balance the transfer out.

Develop mass-balance equations for the reactors, and solve the equations simultaneously for the unknown concentrations (c_1, c_2, c_3) using Gauss-Siedel method (Show two iterations).

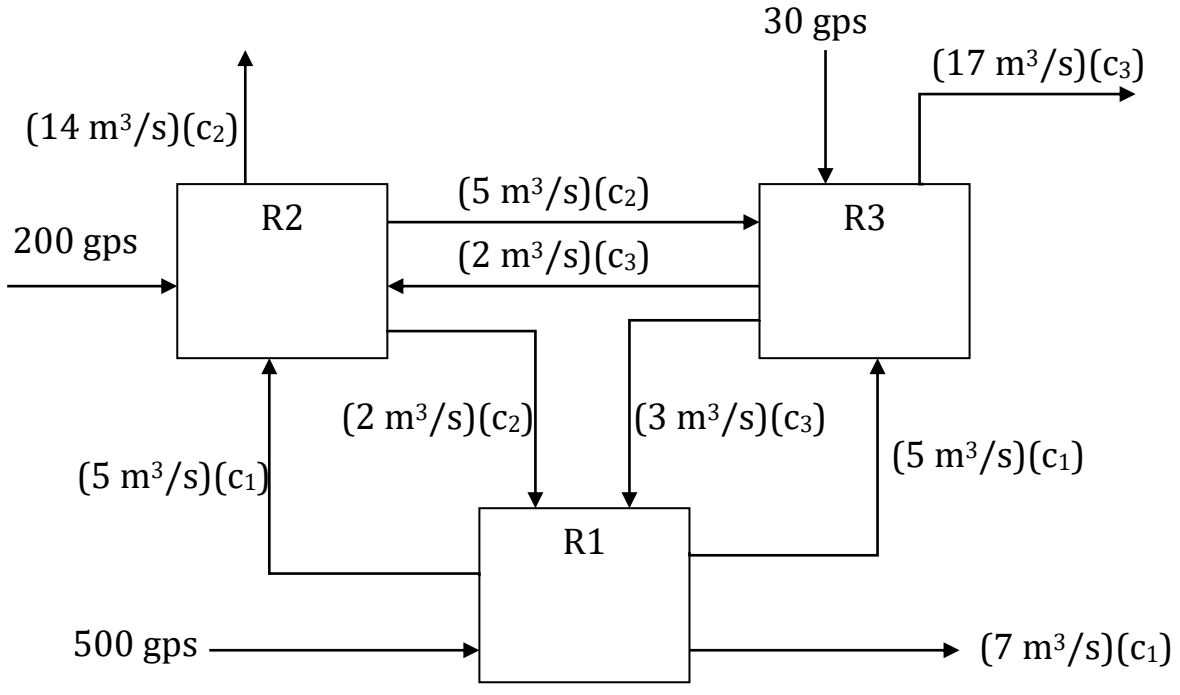

Fig. 2

[(CO2)(Analyse/HOCQ)]

(b) Comment on the criteria based on which one can apply the Gauss-Elimination method for a set of simultaneous equations in the form AX=B, where A is the coefficient matrix, X is the solution matrix and B is the constant matrix.

[(CO)(Remember/LOCQ)]

9 + 3 = 12

Group - D

6. A U-tube manometer (used to measure pressure) (Fig. 3) is initially filled with water, but is exposed to a pressure difference such that the water level on the left side of the U-tube is 0.025 m higher than the water level on the right. At t = 0 there is no movement of the water level in the manometer with the pressure difference suddenly removed. The height of the water level on the left side, y, measured from the mid-plane where L = 0.1 m is the total length of the U-tube, and g = 9.81 m/s2. *(GS 10.33)*

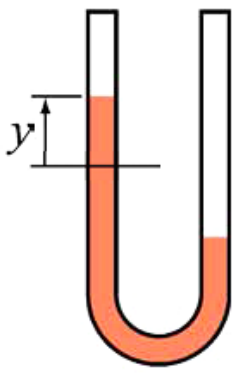

Fig. 3

Considering friction, the first order differential equation modelling the system is given by $L\frac{d^2y}{dt^2} = -0.05\frac{dy}{dt} - 2gy$

(a) Convert the above 2nd order ODE to a set of first order ODEs. State all initial conditions for each ODE based on the data given. (GS 10.33). *[(CO3)(Apply/IOCQ)]*

(b) Calculate value of y(0.1) and y(0.2) and $\left.\frac{dy}{dt}\right|_{t=0.1}$ assuming a time step of 0.1 using Euler Explicit method. *[(CO3)(Apply/IOCQ)]*

(c) Calculate the relative error with respect to the solution obtained in (b) if a time step of 0.2 were taken to calculate the value of y(0.2) and $\left.\frac{dy}{dt}\right|_{t=0.1}$ *[(CO1,CO3)(Apply/IOCQ)]*

(4 + 4 + 4) = 12

7. (a) Derive the ordinary differential equation to predict the height of the water level $y(t)$ (Fig. 4) as a function of time $t$in a tapered funnel with a taper angle $\theta = 45^o$ as shown in figurebelow. The funnel contains water at an initial level H = 150 mm. Water exits the funnel at a velocity of $v_e = \sqrt{2gy}$ where g is acceleration due to gravity. *[(CO3)(Analyse/HOCQ)]*

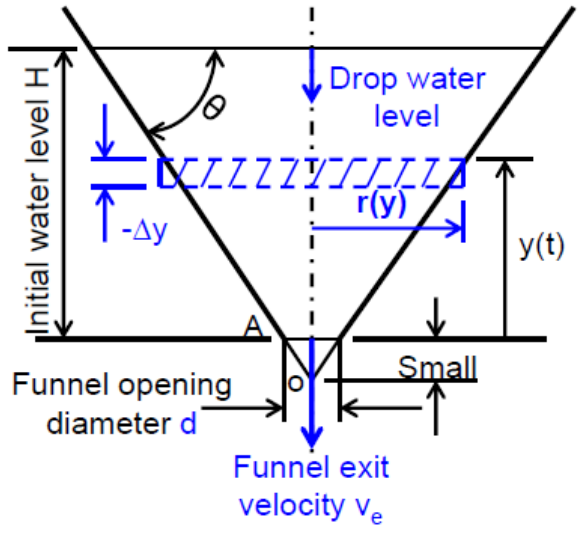

Fig. 4

(b) Use <u>any</u> 2nd order RK method to evaluate the height of water in the funnel after 1 sec if the initial height of water is 150mm. The funnel opening diameter, d = 6mm. Assume a step size of 0.5s. *[(CO3)(Apply/IOCQ)]*

6 + 6 = 12

Group - E

8. (a) Show that for stable iteration during solving a parabolic PDE using Crank-Nicolson scheme, the time step (Δt) is related with spatial step (Δx) as $\Delta t < \frac{1}{\alpha}(\Delta x)^2$. *[(CO3)(Remember/LOCQ)]*

(b) Develop coefficient matrix for an unsteady state heat transfer problem $\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2}$ with the boundaries T(x,0)=300 K, T(0,t)=900 K and T(1,t)=300 K. Use implicit method to develop the algebraic set of equation. Assume boundary temperatures are constant and Δx=0.2. *[(CO3)(Apply/IOCQ)]*

5 + 7 = 12

9. (a) A pharmaceutical company wishes to mix two types of foods in such a way that vitamin contents of the mixture contain at most 8 units of vitamin A and 10 units of vitamin C. Food I contains '2 units/kg' of vitamin A and '1 unit/kg' of vitamin C. Food II contains 1 unit/kg of vitamin A and 2 units/kg of vitamin C. It costs Rs. 50 per kg to purchase Food I and Rs. 70 per kg to purchase Food II. Using SIMPLEX method evaluate the maximum cost of the mixture (Show three iterations). *[(CO5)(Analyse/HOCQ)]*

(b) Maximize the function $f(x,y)=2xy+2x-x^2-2y^2$ using gradient search algorithm with initial guesses x=-1 and y=1 (Show two iterations). *[(CO5)(Apply/IOCQ)]*

7 + 5 = 12

Cognition Level	LOCQ	IOCQ	HOCQ
Percentage distribution	19.79	41.66	38.54

Course Outcome (CO):

After the completion of the course students will be able to

1. identify different computational errors and evaluate them for a given mathematical problem to be solved numerically. Students will be able to know how to perform relative and absolute error in each case.
2. formulate a nonlinear form of the equation and solve non-linear equations for a given linear multivariable problem.
3. create ODE and PDE along with the associated boundary conditions followed by an application of appropriate numerical algorithm for a given engineering problem.
4. calculate numerical integration to find out area under the function curve for a given engineering problem.
5. design constrained and unconstrained optimization problem for a given engineering problem.

**LOCQ: Lower Order Cognitive Question; IOCQ: Intermediate Order Cognitive Question; HOCQ: Higher Order Cognitive Question.*