



Name : .....

Roll No. : .....

Invigilator's Signature : .....

**CS/B.Tech(CHE-New)/SEM-6/CHE-604/2011**

**2011**

**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.*

**GROUP – A**

**( Multiple Choice Type Questions )**

1. Choose the correct alternatives for any *ten* of the following :

$$10 \times 1 = 10$$

- i) If a function  $f(x)$  is real and continuous in the interval  $a < x < b$  and  $f(a) \cdot f(b) < 0$ , then
  - a) there is at least one real root between  $a$  and  $b$
  - b) there is only one real root between  $a$  and  $b$
  - c) there is no root between  $a$  and  $b$
  - d) none of these.
- ii) For an equation like  $x^2 = 0$ , a root exists at  $x = 0$ . The bisection method cannot be applied to solve this equation in spite of the root existing at  $x = 0$  because the function  $f(x) = x^2$ 
  - a) is a polynomial
  - b) has repeated root at  $x = 0$
  - c) is always non-negative



- d) slope is zero at  $x = 0$ .
- iii) In secant method for finding the square root of a real number 'R' from the equation  $x^2 - R = 0$ , the formula is
- a)  $\frac{x_n x_{n-1} + R}{x_n + x_{n-1}}$       b)  $\frac{x_n x_{n-1}}{x_n + x_{n-1}}$
- c)  $\frac{1}{2} \left( x_n + \frac{R}{x_n} \right)$       d)  $\frac{2x_n^2 + x_n x_{n-1} - R}{x_n + x_{n-1}}$
- iv) If for a real continuous function  $f(x)$ ,  $f(a)f(b) < 0$ , then in the range of  $[a, b]$  for  $f(x) = 0$ , there is (are)
- a) one root
- b) indeterminable number of roots
- c) no root
- d) at least one root.
- v) Modified Euler's method is
- a) implicit method      b) explicit method
- c) both of these      d) none of these.
- vi) In Gauss-Jordan method
- a) a variable is eliminated from the rows above the pivot position
- b) a variable is eliminated from the rows below the pivot position
- c) a variable is eliminated from the rows both above and below the pivot position



- d) a variable is eliminated from the pivot position.
- vii) Least square method is used to derive
- a) a curve that maximize the discrepancy between the data points and the curve
  - b) a curve that minimize the discrepancy between the data points and the curve
  - c) a straight line that maximize the discrepancy between the data points and the straight line
  - d) a straight line that minimize the discrepancy between the data points and the straight line.
- viii) Simpson's  $\frac{1}{3}$  rule always requires
- a) even number of ordinates
  - b) odd number of ordinates
  - c) even or odd number of ordinates
  - d) none of these.
- ix) In trapezoidal rule, the order of  $h$  in the total error is
- a) 3
  - b) 4
  - c) 2
  - d) none of these.
- x) When Gauss elimination method is used to solve  $AX = B$ ,  $A$  is transformed to a
- a) unit matrix
  - b) lower triangular matrix
  - c) diagonally dominant matrix



- d) upper triangular matrix.
- xi) Euler's method for solving ODE initial value problem given by the formula  $y_{n+1} = y_n + hy_n$  is a
- a) explicit second order technique
- b) implicit first order technique
- c) explicit first order technique
- d) implicit second order technique.
- xii) A linear second order PDE represented by
- $$a \frac{\partial^2 z}{\partial x^2} + b \frac{\partial^2 z}{\partial x \partial y} + d \frac{\partial^2 z}{\partial y^2} + e \frac{\partial z}{\partial x} + f \frac{\partial z}{\partial y} + gz = h, \text{ where}$$
- $a, b, d, e, f, g, h$  are functions of  $x$  and  $y$  is parabolic when
- a)  $b^2 < 4ad$
- b)  $b^2 = 4ad$
- c)  $b^2 > 4ad$
- d) none of these.

### GROUP – B

#### ( Short Answer Type Questions )

Answer any *three* of the following.  $3 \times 5 = 15$

2. Find the cube root of 12 using bisection method correct up to two decimal places.
3. Solve by Euler's method the following differential equation :
- $$2 \frac{d^2 y}{dx^2} + 3 \frac{dy}{dx} + 5y = 11 e^{-x},$$
- $$y(0) = 7, \frac{dy}{dx} = 13 \text{ at } x = 0.$$



Calculate  $y$  at  $x = 0.5$  with  $h = 0.25$ .

4. Find the root of equation  $x^2 - 5x + 2 = 0$  using Newton-Raphson method in the vicinity of  $x = 1.5$ . Perform up to three iteration.
5. a) State the condition for existence of a unique solution of a first order initial value problem.  
 b) Why is Crank-Nicholson technique considered an improvement over implicit method ? 3 + 2
6. Use Jacobi method of obtain the solution of the following system of equations :

$$x_1 + x_2 + 4x_3 = 9$$

$$8x_1 - 3x_2 + 2x_3 = 20$$

$$4x_1 + 11x_2 - x_3 = 33.$$

### GROUP – C

#### ( Long Answer Type Questions )

Answer any *three* of the following. 3 × 15 = 45

7. a) Develop tri-diagonal matrix algorithm ( TDMA ) and explore its use in solving component material balance and equilibrium relationships in multicomponent multistage distillation column. Develop all the equations for a simple distillation column, having one feed stream and two products ; distillate and bottoms.
- b) Solve the following set of simultaneous equations by Gauss elimination method with partial pivoting and mention the steps clearly :

$$2x_1 - x_2 + x_3 = 7$$

$$x_1 + 2x_2 + x_3 = 0$$

$$3x_1 + x_2 - 2x_3 = -2.$$

8 + 7



8. a) A non-isothermal batch reactor can be modelled by :

$$\frac{dc}{dt} = -e^{\left(-\frac{10}{T+273}\right)} C$$

$$\frac{dT}{dt} = 1000 e^{\left(-\frac{10}{T+273}\right)} C - 10 (T - 20)$$

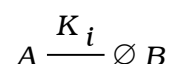
Initially the reactor is at 25°C and concentration of reactant  $C = 1$  gmol/L. Find the concentration and temperature of the reactor at  $t = 20$  min using  $h = 10$  and 4th order Runge-Kutta method.

- b) Use the data given in the following table to fit the 2-D model for diffusion coefficient as function of temperature ( $T$ ) and weight function ( $X$ ).

$T (^\circ\text{C})$	20	20	25	25	30	30
$X$	0.3	0.5	0.3	0.5	0.3	0.5
$D \propto 10^5 \text{ cm}^2/\text{s}$	0.823	0.43	0.973	0.506	1.032	0.561

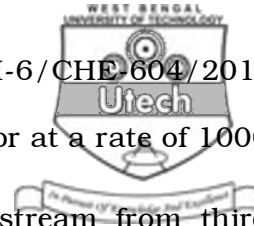
$$\text{Model : } D = C_1 + C_2 T + C_3 X. \quad 8 + 7$$

9. a) A first order irreversible chemical reaction ( in liquid phase ) takes place in a series of three CSTRs arranged as shown below :



The condition of temperature in each reactor is such that the value of  $K_i$  is different in each reactor. Also, the volume of each reactor ( $V_i$ ) is different. The values of  $K_i$  and  $V_i$  are given below :

Reactor	$V_i$ ( lit )	$K_i . h^{-1}$
1	1000	0.1
2	1500	0.1
3	500	0.3



The feed stream enters the first reactor at a rate of 1000 lit./h with an initial concentration of  $C_{AO} = 1$  mol/lit. The flow rate of stream from third CSTR to second one is at the rate of 100 lit/h.

The exit stream flow rate from the third reactor is 1000 lit/h. Assuming steady state, set up the material balance equation for each reactor and solve the set of equations to find the exit concentration ( $C_{A_i}$ ) from each reactor using suitable numerical technique.

b) Write down Taylor's theorem. 13 + 2

10. a) A first order reaction takes place in a tubular reactor. The advection-dispersion equation at steady state is given by  $D \frac{d^2c}{dx^2} - U \frac{dc}{dx} - kc = 0$ .

The following boundary conditions hold :

$$\text{At } x = 0, QC_{in} = QC_o - DA_c \frac{dc_o}{dx} \quad \text{and at } x = 5 \text{ cm, } DA_c \frac{dc_o}{dx} = 0.$$

Solve for steady state concentration levels when diffusivity  $D = 2 \text{ cm}^2 / \text{s}$ , velocity of fluid  $U = 1 \text{ cm/s}$ ,  $\Delta x = 2.5 \text{ cm}$ ,  $k = 0.2 \text{ s}^{-1}$  and  $C_{in} = 150 \text{ gmol/cc}$ .

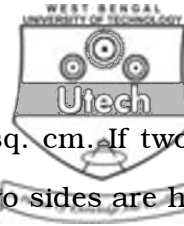
- b) Explain why Gauss-Seidel iterative method is not suitable for solving the following system of equations :

$$x + y + z = 3$$

$$x + y - z = 1$$

$$x - y + z = 1.$$

10 + 5



11. a) Consider a steel plate size of  $15 \times 15$  sq. cm. If two of the sides are held at  $200^{\circ}\text{C}$  and other two sides are held at  $0^{\circ}\text{C}$ , what is the steady state temperature at interior point assuming grid size of  $5 \times 5$  sq. cm. ( solve the set of equations by Gauss-elimination method ) ?
- b) Apply Crank-Nicholson method to solve the unsteady state conduction problem :

where, IC :  $T(x, 0) = 100(1 - x^2)$

BC :  $T(0, t) = 100.0$

$T(1, t) = 0.0$

Assuming,  $M = (\Delta x)^2 / \Delta t / \alpha = 2.5$  and  $\alpha = 1.0$  and the rectangular heat slab consists of four equal slices, compute the temperature profile with length. 5 + 10

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