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 $f(a).f(b) < 0$, 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) $\dfrac{x_n x_{n-1} + R}{x_n + x_{n-1}}$

b) $\dfrac{x_n x_{n-1}}{x_n + x_{n-1}}$

c) $\frac{1}{2}\left(x_n + \dfrac{R}{x_n} \right)$

d) $\dfrac{2x_n^2 + x_n x_{n-1} - R}{x_n + x_{n-1}}$.

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-Jordon 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

$$a\frac{\partial^2 z}{\partial x^2} + b\frac{\partial^2 z}{\partial x \partial y} + d\frac{\partial^2 z}{\partial y^2} + e\frac{\partial z}{\partial x} + f\frac{\partial z}{\partial y} + gz = h,$$ 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 :

$$2\frac{d^2y}{dx^2} + 3\frac{dy}{dx} + 5y = 11e^{-x},$$

$$y(0) = 7, \frac{dy}{dx} = 13 \text{ at } x = 0.$$

Calculate y at $x = 0{\cdot}5$ with $h = 0{\cdot}25$.

4. Find the root of equation $x^2 - 5x + 2 = 0$ using Newton-Raphson method in the vicinity of $x = 1{\cdot}5$. 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 an 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 (°C)	20	20	25	25	30	30
X	0·3	0·5	0·3	0·5	0·3	0·5
D ∞ 10^5 cm^2/s	0·823	0·43	0·973	0·506	1·032	0·561

Model : $D = C_1 + C_2 T + C_3 X$. 8 + 7

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

$$A \overset{K_i}{\overline{\qquad}} \varnothing\, B$$

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 $\left(C_{A_i} \right)$ 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 :

At $x = 0$, $QC_{\text{in}} = QC_o - DA_c \frac{dc_o}{dx}$ and at $x = 5$ 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 $U = 1$ cm/s, $\Delta x = 2{\cdot}5$ cm, $k = 0{\cdot}2\ \text{s}^{-1}$ and $C_{in} = 150$ 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 ∞ 15 sq. cm. If two of the sides are held at 200°C and other two sides are held at 0°C, what is the steady state temperature at interior point assuming grid size of 5 ∞ 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, $M = (\Delta x)^2 / \Delta t / \alpha = 2{\cdot}5$ and $\alpha = 1{\cdot}0$ and the rectangular heat slab consists of four equal slices, compute the temperature profile with length. 5 + 10