Name : .....

Roll No. : .....

Invigilator's Signature : .....

CS/B.TECH(CHE)/SEM-6/CHE-604/2012

2012

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) The Secant method formula for finding the square root of a real number 'R' from the equation $x^2 - R = 0$ is

   a) $\dfrac{x_i x_{i-1} + R}{x_i + x_{i-1}}$ b) $\dfrac{x_i x_{i-1}}{x_i + x_{i-1}}$

   c) $\dfrac{1}{2}\left(x_i + \dfrac{R}{x_i}\right)$ d) $\dfrac{2x^2{}_i + x_i x_{i-1} - R}{x_i + x_{i-1}}$.

   ii) 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) undeterminable number of roots

   c) no root

   d) at least one root.

iii) Huen's method is

a) The method having more Truncation error than Euler's method

b) 1st order Runge-Kutta Method

c) not an iterative method

d) 2nd order Runge-Kutta Method

iv) A heated rectangular slab has one of its sides held at constant heat flux. The other three sides are held at constant temperatures of 50°, 25° and 75° C. Considering 3 interior nodes in the x and y direction each, numerical differencing scheme will generate a

a) 9 × 9 matrix b) 12 × 9 matrix

c) 9 × 12 matrix d) 12 × 12 matrix.

v) The Explicit scheme for solving the heat conduction equation is both convergent, stable and will not have oscillating solutions if

a) $\Delta t \leq \frac{\Delta x^2}{k}$ b) $\Delta t \leq \frac{\Delta x^2}{2k}$

c) $\Delta t \leq \frac{\Delta x^2}{4k}$ d) $\Delta t \leq \frac{2\,\Delta x^2}{k}$.

vi) Round off the number 86·23852753 up to 5 significant figures

a) 86·238 b) 86·239

c) 86·23852 d) 86·23853 .

vii) Runge-Kutta formula has a Truncation error, which is of the order of

a) h^2 b) h^4

c) h^5 d) none of these.

viii) Tridiagonal matrix algorithm (TMDA) is a special case of

a) Secant Method

b) Gauss-Seidel Method

c) Newton-Raphson method

d) Gauss-elimination method.

ix) Crank-Nicholson formula is called

a) an explicit method

b) an explicit method

c) semi-implicit method

d) semi-explicit method.

x) Which of the following method is used for solving boundary value problem during numerical solution of ordinary differential equation ?

a) Euler's method b) Heun's method

c) Runge-Kutta method d) Finite difference.

xi) Successive over-relaxation is used

a) as a modified Gauss-Seidel technique

b) in finding roots of polynomial

c) in finding constants for Newton interpolation

d) for faster convergence in Newton-Raphson.

xii) 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.

GROUP – B

(Short Answer Type Questions)

Answer any *three* of the following. 3 × 5 = 15

2. Find the thermal conductivity (k) of propane by using Lagranges interpolation formula at $1{\cdot}013 \times 10^4$ kN/m^2 and 99 °C from data given in the following table at the same pressure :

Temperature, T°C	68	87	106	140
Thermal conductivity, k(W/m K) at $1{\cdot}013 \times 10^4$ kN/m^2	0·0853	0·0774	0·0699	0·0618

3. Fit the curve $y = ax^{\prime}$ by curve fitting method for the following data points (1, 1200), (2, 900), (3, 600), (4, 200), (5, 100), (6, 50).

4. Solve the differential by Euler's method $dy/dx = x^2y$, with the initial condition $y(0) = 1$. Find $y(0{\cdot}3)$. Compare your result with the analytical solution.

5. Solve the following system of equation with partial pivoting :

$$2x - 6y - z = -38$$

$$-3x - y + 7z = -34$$

$$-8x - y + 2z = -20$$

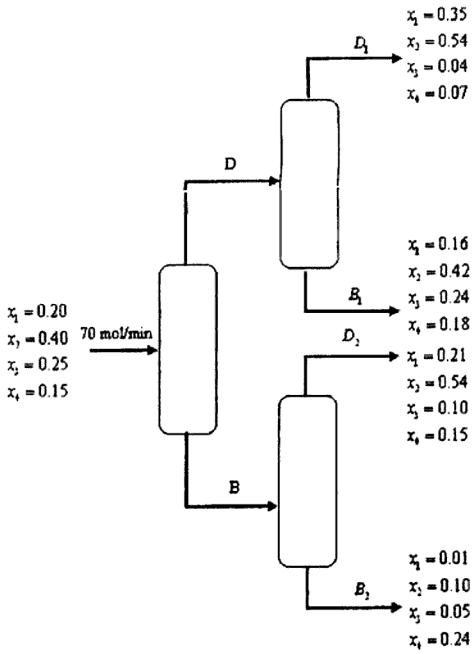
6. Evaluate the following integral using Simpson's $\frac{1}{3}$rd rule $\int_0^4 \left(1 - e^{-2x}\right) dx$ (Taking $n = 0{\cdot}5$).

GROUP – C

(Long Answer Type Questions)

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

7. a) Benzene(1), toluene (2), styrene (3) and xylene (4) are to be separated in the sequence of distillation column shown in Fig. Determine molar flow rates of streams D_1, B_1, D_2 and B_2. The composition of the feed and the streams D_1, B_1, D_2 and B_2 is shown in Fig. Also determine the molar flow rates and composition of B and D. The molar flow rate of the stream is 70 mol/min.



b) Find a real root equation $x^2 - x - 1 - 0$ by Bijection method up to 4 signification figures. 10 + 5

8. a) When a microorganism is grown in a batch fermentor under carefully controlled condition, the cell reproduction rate can be modelled as :

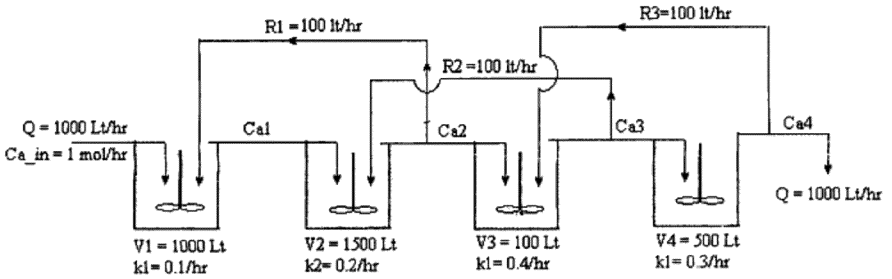
$\frac{dy_1}{dt} = b_1 y_1 \left(1 - \frac{y_1}{b_2}\right)$ where y_1 is the concentration of cells expressed as percentage dry weight. In addition, the rate of production of the microorganism, y_2 has been found to obey $\frac{dy_2}{dt} = b_3 y_1 - b_4 y_2$ where y_2 is the units of microorganism per mL. Given that $b_1 = 0 \cdot 1$, $b_2 = 4$, $b_3 = 0 \cdot 02$ and $b_4 = 0 \cdot 02$, evaluate y_1 and y_2 at time = 50 hours if the initial values of y_1 is 0·18 per cent dry weight and y_2 is 0·2 units/ml.

b) It is desired to solve the following equation :

$f(x) = x^3 - 5x^2 + 7x - 3 = 0$ by Newton-Raphson Method, but it is observed that the good initial guess like $x^{(0)} = 0$ requires a large number of iteration to find one root x = 1. Justify the above observation and suggest some modification to reduce the number of iteration.

10 + 5

9. a) A set of isothermal CSTR is operated in series with recycle. Find the outlet concentrations from each of CSTR.



b) Illustrate the concept of truncation error. What is the basis of obtaining the initial guess for any iterative method to be applicable for practical problem ? 10 + 5

10. The catalytic gas phase reaction between components A and B is occurring reversibly in a catalyst layer at a particular point in a monolithic reactor.

$2A \leftrightarrow B$

The catalytic reaction rate expression for reactant A is given by $r_A = -k(C_A{}^2 - C_B / K_C)$

where the rate is in g-mole /cm^3/s, the rate constant k has been determined to be 8×10^4 in cm^3/s. g-mole, and the equilibrium constant is known to be $K_C = 6 \times 10^5 cm^3$/g-mol. The catalytic layer as a thickness of L = 0·2 cm, and the effective diffusivity of A in B, for this layer is $D_e = 0 \cdot 01$ cm^2/s. The reactant mixture contains only gases A and B, so only binary gas diffusion need be considered. The total concentration of A and B is $C_T = 4 \times 10^{-5}$ g-mol/cm^3. Calculation of the effectiveness factor requires consideration of the simultaneous diffusion of both components along with material balance involving the reversible reaction rate expression.

Use an implicit finite difference technique to calculate the effectiveness factor for the given reaction and summarize C_A and N_A in a table at 10 equally spaced intervals within the catalytic layer. The reactant concentration at the surface of the layer are known to be $C_{AS} = 3 \times 10^{-5}$ g-mol/cm^3 and $C_{BS} = 1 \times 10^{-5}$g-mole/$cm^3$.

11. a) Water is following through a pipe line 6 cm in diameter. The local velocities at various radial positions are given below:

u, cm/s	2·00	1·94	1·78	1·50	1·11	0·61	0·00
r, cm	0	0·5	1·0	1·5	2·0	2·5	3·0

Estimate the average velocity $\bar{u}$ by Simpson's $\frac{2}{3}$rd rule .

b) The operation of a constant density plug flow reactor for the production of a substance by an enzymatic is described by the equation : $\frac{V}{F} = -\int_{C_{in}}^{C_{out}} \frac{K}{k_{\max} C} + \frac{1}{k_{\max}}\, dC$ where V is volume of the reactor, F is the flow rate of the reactant, C. C_{in} and C_{out} are the concentrations of reactants entering and leaving the reactor respectively and K and $k_{\max}$ are constants. For a 500L reactor, with an inlet concentration of C_{in}=0·5 M and inlet flow rate of 40 L/s, $k_{\max} = 5 \times 10^{-3} s^{-1}$ and K = 0·1 M, find the concentration of C at the outlet of the reactor.