NUMERICAL METHODS IN CHEMICAL ENGINEERING
(CHEN 3104)

Time Allotted : 3 hrs **Full Marks : 70**

Figures out of the right margin indicate full marks.

Candidates are required to answer Group A and any 5 (five) from Group B to E, taking at least one from each group.

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

Group – A
(Multiple Choice Type Questions)

1. Choose the correct alternative for the following: **10 × 1 = 10**

(i) Chopping of a decimal number yields an absolute error that is ____ than rounding it
(a) higher (b) lower
(c) same (d) none of above.

(ii) The condition number of the function sin(x) at x= 0.785 for a perturbation of $\Delta x=0.001$ is
(a) around 3 (b) around 2
(c) around 1.5 (d) around 1.

(iii) The second order Taylor series expansion of *f(x)* around $x = x_i$ will have terms containing
(a) $f(x_i)$ (b) a and c
(c) $f''(x_i)$ (d) a or c.

(iv) The 0th order approximation of the expansion series of $e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + ...$ around x = 2 is
(a) 0 (b) 2
(c) 1 (d) none of above.

(v) If a function f(x) has four roots between the lower bound x_l and and the upper bound x_u, then
(a) $f(x_l)\, f(x_u) = 0$ (b) $f(x_l)\, f(x_u) < 0$
(c) $f(x_l)\, f(x_u) > 0$ (d) $f(x_l)\, f(x_u) <= 0$.

(vi) In LU decomposition, if [L] and [U] are the lower and upper triangular matrix decomposition of [A] in $[A]\underline{x} = \underline{b}$, then which of the following is true
(a) $[U]\underline{x} = \underline{b}$ (b) $[L]\underline{x} = \underline{b}$
(c) $[A]\,[U]\underline{x} = \underline{b}$ (d) $[L]\,[U]\underline{x} = \underline{b}$.

(vii) Transient heat conduction in a cylindrical rod kept at uniform temperature at both ends can be mathematically modelled by a partial differential equation which is purely

(a) elliptic (b) hyperbolic
(c) parabolic (d) none of above.

(viii) Heun's method of numerically solving an ODE
(a) provides more inaccurate solutions than Euler method
(b) is a second order RK method
(c) a first order RK method
(d) none of above.

(ix) To solve boundary value problems in ODE we require
(a) one initial condition and one boundary condition
(b) two boundary condition
(c) two initial condition
(d) one boundary condition only.

(x) The directional derivative ∇f of a function $f(x,y)=x^2y$ at the point (2,2) is given by

(a) 4i+ 8j (b) 2i+ 4j
(c) 4i+ 4j (d) 8i+ 4j.

Group – B

2. (a) The following data was obtained when the stopping distance d of a car on a wet road was measured as a function of the speed v when the brakes were applied:

v (km/h)	12.5	25	37.5	50	62.5	75
d (km)	20	59	118	197	299	420

Fit cubic splines through above data. Write out the algebraic equation for all spline coefficients and arrange in matrix form (**A**x=b). You do not need to solve the linear system.

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3. (a) The amount of water in air measured at various temperatures at 100% humidity is displayed in the following table:

T (^oC)	0	10	20	30	40
m_{water} (g/kg of air)	5	8	15	28	51

Use Newton interpolation using all data points to predict the value of water mass in air at 35^oC.

(b) State two major difference between Lagrange and Newton interpolation.

8 + 4 = 12

Group – C

4. (a) Carry out the first three iterations of the solution of the following system of equations using the Gauss-Seidel iterative method. For the first guess of the solution, take the value of all the unknowns to be zero. Also calculate the convergence criterion for each iteration.

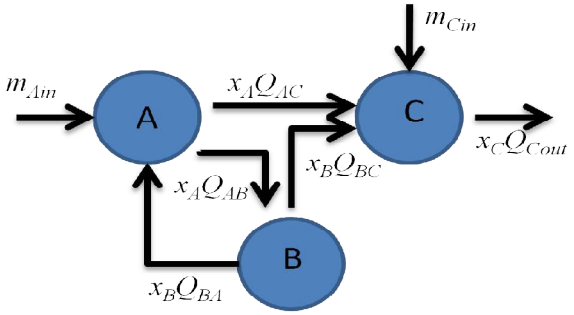
$$8x_1 + 2x_2 + 3x_3 = 51$$
$$2x_1 + 5x_2 + x_3 = 23$$
$$-3x_1 + x_2 + 6x_3 = 20$$

Will you get converged solutions?

(b) Calculate the condition number of the matrix $\begin{bmatrix} 10 & -2 \\ 1.5 & -3.85 \end{bmatrix}$. Is the system well-conditioned?

8 + 4 = 12

5. (a) The chemical engineering process application (shown in figure below) involves three chemical reactors A, B, and C. At steady state, the concentrations of a particular species *n* in each reactor has the values x_A , x_B, and x_C in units of mg/m³. If the flow rates from reactor *i* (A, B, or C) to reactor *j*(A, B, or C) is denoted as Q_{ij} (units of m³/s), then the mass flow rate of species *n* from reactor *i* to reactor *j* is x_iQ_{ij} (units of mg/s). Since this chemical species is conserved (i.e., neither produced nor destroyed) conservation of mass (of the species) for each reactor must hold. For the process shown in the figure, Q_{AB} = 40 m³/s, Q_{AC} = 80 m³/s, Q_{BA} = 60 m³/s, Q_{BC} = 20 m³/s, Q_{cout} = 150 m³/s, m_{Cin} = 195 mg/s, and m_{Ain} = 1320mg/s.



Write down the mass continuity equations for each reactor and develop the equations in the form [A]x = b.

(b) Solve the system to find the concentrations x_A , x_B, and x_C in each reactor.

4 + 8 = 12

Group – D

6. Consider the cylindrical water tank. The tank is being filled at the top, and water flows out of the tank through a pipe that is connected at the bottom. The rate of change of the height, *h*, of the water in tank is given by

$$\rho A_{\tan k}\frac{dh}{dt} = K_1 + K_2 Sin(5Ct)Cos(Ct) - \rho A_{pipe}\sqrt{2gh}$$

Given that $A_{\tan k}$=3.13m^2, A_{pipe}=0.06 m^2, C=π/12, K_1=300 kg/s, K_2=1000kg/s and ρ=1000kg/m^3 and g = 9.81 m/s^2. Determine the height of water in the tank as a function of time for 50s if the initial water height was 3m. Choose time steps of 25s. Use any 2nd order RK method.

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7. Consider the following second-order ODE:

$\frac{d^2y}{dx^2} = e^{-xy}$ from *x = 0* to *x = 1* with *y(0)=0* and $\left.\frac{dy}{dx}\right|_{x=0} = 1$

Use 2nd order Heun's method for two steps $\Delta x = 0.2$

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Group – E

8. (a) A long thin rod of length 20 cm is held at a constant temperature of 80^{o}C at one end. The other end of the rod is kept at 20 ^{o}C. The rod is initially at 20 ^{o}C . The density and thermal conductivity of copper rod is 8.96g/cm^3 and 0.99 cal/(s.cm. ^{o}C). Write out the differential form of the governing equation. Use explicit method with 3 internal grid points. Formulate the equations at every internal grid points using appropriate boundary conditions.

(b) Use the above equations to calculate the temperature profile along the rod at the end of 2 sec.

8 + 4 = 12

9. (a) A computer equipment manufacturer produces scanners and printers. The resources need for producing the devices and the corresponding profits are provided in table below :

Device	Capital (Rs/unit)	Labor(hr/unit)	Profit(Rs/unit)
Scanner	21000	20	35000
Printer	28000	10	28000

Formulate the optimization problem completely.

(b) Solve using simplex method.

4 + 8 = 12

Department & Section	Submission Link
CHE	https://classroom.google.com/c/MTIyMDYwODU0NTU1/a/MjcwOTgyNTM0OTcw/details