Reg. No.										

MANIPAL INSTITUTE OF TECHNOLOGY

MANIPAL

(A constituent unit of MAHE, Manipal)

B.TECH. (CHEMICAL ENGINEERING)

MAKE UP EXAMINATIONS, Dec 2018

SUBJECT:COMPUTATIONAL METHODS IN CHEMICAL ENGINEERING [CHE 3105]

REVISED CREDIT SYSTEM,

Time: 3 Hours **Instructions to Candidates** **MAX MARKS: 50**

- Answer all questions **FULLY**.
- Missing data may be suitable assumed.

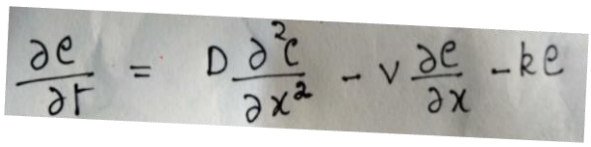
1A	Solve for X by Gauss Elimination method when AX =B A>> 2 3 1 4 B>> 22 1 2 3 2 15 3 1 2 3 26 3 4 5 3 26	**4**
1B	$f(x)= xe^x - \cos(x) =0$ Solve using Newton Raphson method. Initial guess is 0.6.Make 3 iterations	**3**
1C	$0 = \frac{1}{\sqrt{f}} + 2.0 \log\left(\frac{\varepsilon}{3.7D} + \frac{2.51}{Re\sqrt{f}}\right)$ Calculate the friction factor with above equation using regular Falsi method if ϵ/D =0.0001 and Re =10,000. Use lower and upper limits as 0.02 and 0.05 respectively. Make 3 iterations.	**3**

2A	Solve by RK4 method, the equation $dy/dx = 3e^{-x}-0.4y$ Initial condition is that at x=0, y= 5, Take step size as 1.5 , Find y at x= 6	**6**
2B	The specific heat of gas as a function of temperature is given $Cp = 0.4 + \frac{18}{T+40}$ KJ/kg. The temperature of the gas is increased from $T_1 = 10^0C$ to $T_2 = 50^0C$ by the addition of heat at constant pressure. The heat added to the gas is given by the expression: $Q = \int_{T1}^{T2} Cp\, dt$ Determine the total heat added to the gas using Simpsons 1/3 rule, make 8 intervals.	**4**

3A	The rate of an enzymatic reaction is given by the expression: $r = \frac{k[S]}{K_m+[S]}$ The k and Km can be estimated by linear regression by defining x =1/S and y =1/r, Find the values of K_m and k. Find the value of R^2 of the linear fitting. [S] 1.233 0.540 0.442 0.258 0.198 0.162 0.130 0.128 r 5.970 3.319 2.253 2.547 1.493 1.182 1.095 0.869	**8**

3B	The vapor pressure of water increase with temperature. The values are tabulated below. T °C: 30, 40, 50, 60 p_v (mm Hg): 31.8, 55.3, 92.5, 149.4 Find the vapor pressure at 45 ^{0}C using Newton's forward interpolation	**2**

4A	Solve the system of simultaneous non-linear equations using Newton-Raphson method $x^2+y=11$ $x+y^2=7$ Initial guess $x_o = 3.5$, $y_o = -1.8$. Make 1 iterations.	**4**
4B	Solve by RK4 method and find value of y and z at x =0.2 $dy/dx = x+z$ $dz/dx = x-y^2$ Step size $\Delta x = 0.1$. Initial condition is that at x=0, y=2, z=1	**6**

5	Solve the equation for flow with reaction in a PFR using finite difference implicit method  where C is concentration in water (mol/L), t is time (s), v is pore water flow velocity (m/s), x is distance (m), D is the hydrodynamic dispersion coefficient (m^2/s), k is the first order reaction constant The length of reactor is 1 m. dx= 0.25 m, dt =1 s. At time t=0, the initial concentration is 0 at all nodes except left boundary where the boundary condition is concentration is 1 mol/L. The other end of the rod has zero dispersion boundary condition. Pore Velocity = 0.25 m/s, k=0.3 s^{-1}, Dispersion coefficient D = 0.3m/s^2, Take dx =0.25 m, Find the concentrations at the nodes at time =1 seconds	**10**