Name:

Enrolment No:

UNIVERSITY OF PETROLEUM AND ENERGY STUDIES

End Semester Examination, December 2018

Program: B. Tech APE GAS **Semester: V**
Subject (Course): Numerical Methods in Chemical Engineering **Max. Marks: 100**
Course Code : MATH 311 **Duration: 3 Hrs.**
No. of page/s: 3

Instruction(s):

(a) Assume the appropriate value of missing data if any.

(b) Mathematical and engineering terms have their usual meanings.

SECTION A (12×5 =60 M)

ANSWER ALL QUESTIONS (Q 5 has an internal choice)

<table>
<tr><td>S. No.</td><td></td><td>Marks</td><td>CO</td></tr>
<tr><td>Q 1</td><td>The “divide and average” method, an old-time method for approximating the square root of any positive number S, can be formulated as

$$x_{i+1} = \frac{1}{2}\left(x_i + \frac{S}{x_i}\right)$$

Prove that this formula is based on the Newton-Raphson algorithm. Find the square root of 2 using this algorithm, with initial guess x = 1.</td><td>12</td><td>CO2</td></tr>
<tr><td>Q2</td><td>A river is 80 meters wide. The depth <i>D</i> in meters at a distance <i>x</i> meter from one bank is given by the following table. Calculate the cross section area of the river using (a) Simpson’s 1/3 rule (b) Simpson’s 3/8 rule.
<table>
<tr><td><i>x</i> in meter</td><td>0</td><td>10</td><td>20</td><td>30</td><td>40</td><td>50</td><td>60</td><td>70</td><td>80</td></tr>
<tr><td><i>D</i> in meter</td><td>0</td><td>4</td><td>7</td><td>9</td><td>12</td><td>15</td><td>14</td><td>8</td><td>3</td></tr>
</table></td><td>12</td><td>CO3</td></tr>
<tr><td>Q 3</td><td>Use the Gauss –Siedel method with successive over-relaxation (w= 1.2), to find the approximate solution of the following system of equations with initial guess $\mathbf{X}^{(1)} = [0\ \ 0\ \ 0]^T$. Carry out the <u>TWO</u> iterations.

$$\begin{bmatrix} 2 & -6 & -1 \\ -3 & -1 & 7 \\ -8 & 1 & -2 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} -38 \\ -34 \\ -20 \end{bmatrix}$$</td><td>12</td><td>CO1</td></tr>
</table>

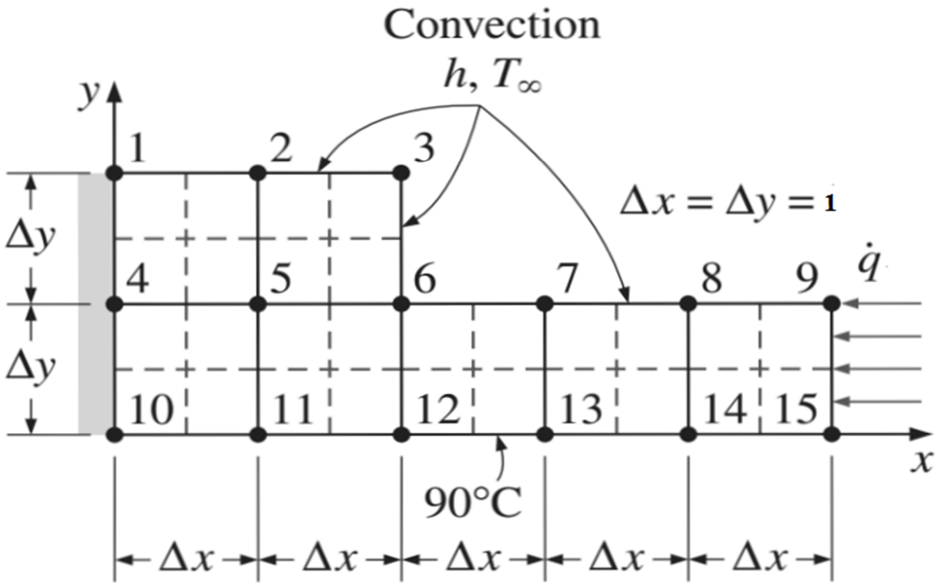
Q 4	The molar volume of a fluid can be estimated using the van der Walls equation of state, $(P + \frac{a}{v^2})(v - b) = RT$ Where, the thermodynamic terms have their usual meanings and a, b are van der Walls constants, which depends on the critical properties of the fluid as, $a = \frac{27R^2T_c^2}{64P_c}$ and $b = \frac{RT_c}{8P_c}$. Write a MATLAB code to estimate the molar volume of saturated liquid water and saturated water vapor at 1 atm pressure and 373 K using the Newton Raphson method (you are not required to obtain the solution). For water $T_c = 647.1K$ and $P_c = 220.55$ bar.	**12**	**CO6**
Q 5	Find the value of y at x = 1.1 using the fourth order Runge- Kutta method, $\frac{dy}{dx} = y^2 + xy$, $y(1) = 1$ and step size h = 0.05. OR Solve the first order ordinary differential equation from t=0 to t=1 $\frac{dy}{dt} + 1.5y - yt^3 = 0$; with condition y(0)=1, using modified Euler's method with step size 0.5. You are required to perform only one iteration to correct the value of y (0.5) and y(1).	**12**	**CO4**

SECTION B (20×2 =40 M)

ANSWER ANY TWO QUESTIONS

Q 6	Suppose the following chemical reactions take place in a continuous stirred tank reactor (CSTR), $A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B \underset{k_4}{\overset{k_3}{\rightleftharpoons}} C$ Where the rate constants are as follows, $k_1 = 1$ min^{-1}, $k_2 = 0$ min^{-1}, $k_3 = 2$ min^{-1},	**20**	**CO4**

	$k_4 = 3$ min^{-1}. The initial charge to the reactor is all *A*, so the initial conditions are (in mol/L), $C_{AO} = 1, C_{BO} = C_{CO} = 0$. An unsteady-state mass balance on each component leads to the following set of ODEs: $\frac{dC_A}{dt} = -k_1C_A + k_2C_B$ $\frac{dC_B}{dt} = k_1C_A - k_2C_B - k_3C_B + k_4C_C$ $\frac{dC_C}{dt} = k_3C_B - k_4C_C$ Use explicit Euler method to find the concentration of each component after 0.03 min with a step size of 0.01 min.		
Q 7	Let us consider an L- shaped structure (thermal conductivity, $k = 5 \quad W/m-K$) in which heat is generated uniformly at a constant rate of $\dot{g} = 5\times10^6 W/m^3$ as shown in the figure below. The steady state heat conduction takes place in the structure as per the equation $\frac{\partial^2 T}{dx^2} + \frac{\partial^2 T}{dy^2} + \frac{g}{k} = 0$. The left surface is insulated and the bottom surface is at a uniform temperature of 90 ^{o}C. The entire top surface is subjected to convection to the ambient air at 25 ^{o}C with a convective heat transfer coefficient of *h* = 75 W/m^2°C. The right surface is subjected to a uniform heat flux of 4500 W/m^2. Discretize the equation using step size $\Delta x = \Delta y = 1$ cm. Formulate the problem into the solvable form of a system of linear equation Ax = b. You are not required to obtain the solution.	**20**	**CO5**

			
Q 8	Heat transfer in a straight fin of the uniform cross section is given as, $\frac{d^2\theta}{dx^2} - m^2\theta = 0$ $x=0, \quad \theta = 1$ $x=1, \quad \frac{d\theta}{dx} = -(Bi)\theta$ Where θ is the dimensionless temperature at any position in the fin, x is the dimensionless location, Bi is the dimensionless Biot number, and m^2 is the product of Bi and a dimensionless group involving the fin dimensions. Obtain the set of algebraic equations to be solved using the finite difference technique with step size 0.25. You are not required to obtain the solution	**20**	**CO4**