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UNIVERSITY OF PETROLEUM AND ENERGY STUDIES

End Semester Examination, December 2017

Program: B. Tech APE GAS

Subject (Course): Numerical Methods in Chemical Engineering

Course Code : MATH 311

No. of page/s: 3

Semester: V

Max. Marks: 100

Duration: 3 Hrs.

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

1. Suppose the temperature of a metal rod of length 10 m has been measured to be 0 °C and 10 °C at each end, respectively. Find the temperatures x_1 , x_2 , x_3 , and x_4 at the four points equally spaced with the interval of 2 m, assuming that the temperature at each point is the average of the temperatures of both neighboring points. Formulate the problem into a system of linear equations, solve those equations using Gauss- Siedel algorithm with initial guess, $x = [1.8 \ 3.8 \ 5.8 \ 7.8]^T$. Carry out the three iterations.
2. The vapour pressure (bar) data for acetone as a function of temperature (K) is given below, ($259.2 \leq T \leq 320.5$).

T (K)	259.2	273.4	290.1	320.5
P ^{sat} (bar)	0.04267	0.09497	0.21525	0.74449

Using Lagrangian interpolation, obtain an appropriate third degree polynomial for the vapour pressure of acetone.

3. The pressure volume data for a thermodynamic process in a closed system is given as follows

P (kPa)	336	294.4	266.4	260.8	260.5	249.6
Volume(m ³)	0.5	2	3	4	6	8

Determine the work produced (kJ) in an isothermal process using (a) trapezoidal rule (b) Simpson's 1/3 rule (c) Simpson's 3/8 rule.

4. (a) Use the Newton-Raphson method, with 3 as starting point, to find a fraction that is within 10^{-4} of $\sqrt{10}$.
 (b) Discuss the condition for rate of convergence of Newton-Raphson algorithm using fixed point iteration method.
5. Solve the second order ordinary differential equation from $t=0$ to $t=2$
 $\frac{dy}{dt} + 1.5y - yt^3 = 0$; with conditions $y(0)=1$,
 (a) Using 1st order Euler's method with step size 0.25
 (b) Using 1st order Euler's method with step size 0.50

Compare the truncation error and comment on the results

SECTION B (20×2 =40 M)

ANSWER ANY TWO QUESTIONS

6. Consider a series reaction $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ carried out in a batch reactor. The differential equation for component A is,

$$\frac{dC_A}{dt} = -k_1 C_A$$
 for component B is,

$$\frac{dC_B}{dt} = k_1 C_A - k_2 C_B$$
 and for component C ,

$$\frac{dC_c}{dt} = k_2 C_B$$
 The initial condition is: at $t = 0$, $C_A = 1, C_B = 0$, and $C_c = 0$. The rate constants are $k_1 = k_2 = 1 \text{ sec}^{-1}$. Use the fourth order Runge - Kutta method to determine the concentration of A, B and C up to 6 sec, using step size of 2 sec.
7. Consider a large uranium plate of thickness $L = 4 \text{ cm}$ and thermal conductivity $k = 28 \text{ W/m } ^\circ\text{C}$ in which heat is generated uniformly at a constant rate of $\dot{g} = 5 \times 10^6 \text{ W} / \text{m}^3$. One side of the plate is maintained at 0°C by iced water while the other side is subjected to convection to an environment at $T = 30^\circ\text{C}$ with a heat transfer coefficient of $h = 45$

$W/m^2\text{°C}$. Considering a total of three equally spaced nodes in the medium, two at the boundaries and one at the middle, estimate the exposed surface temperature of the plate under steady conditions using the finite difference approach.

The heat transfer equation can be given as, $\frac{d^2T}{dx^2} + \frac{\dot{g}}{k} = 0$

Assumptions (a) Heat transfer is one-dimensional since the plate is large relative to its thickness. (b) Thermal conductivity is constant. (c) Radiation heat transfer is negligible.

8. Let us consider a L- shaped structure (thermal conductivity, $k = 15W / m - K$) as shown in the figure below. The steady state heat conduction takes place in the structure as

per the equation $\frac{\partial^2T}{dx^2} + \frac{\partial^2T}{dy^2} = 0$. The left surface is insulated and the bottom surface is at

uniform temperature of 90 °C . The entire top surface is subjected to convection to the ambient air at 25 °C with a convective heat transfer coefficient of $h = 75 W/m^2\text{°C}$. The right surface is subjected to uniform heat flux of $4500 W/m^2$. Discretize the equation using step size $\Delta x = \Delta y = 1\text{ cm}$. Formulate the problem in to the solvable form of system of linear equation $Ax=b$. You are not required to obtain the solution.

