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B.Tech. (ChE), End Term Examination, Autumn Semester 2022-2023

CHN-323 Computer Applications in Chemical Engineering **Max Marks: 70, Time: 180 mins**

INSTRUCTIONS:

1. Attempt all questions. Answer all parts of a question at single place.
2. Please check all pages of question paper and report the discrepancy, if any.
3. Return the MCQ sheet within first 30 min of the exam; each MCQ is for 0.5 marks.
4. Make suitable assumptions wherever necessary.

Question 1:

In an experiment, the following data (16 pairs of x and y) were obtained.
x = [35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50]
y = [405 285 207 154 118 93 74 60 49 41 35 30 26 22 20 17]

The x and y variables are related via the following equation

$$y = \exp\left(a + \frac{b}{x - c}\right)$$

You are asked to determine values of parameters a, b and c. Convert this parameter estimation problem into an optimization problem. Finally, write a MATLAB program to solve the optimization problem. **[10 marks]**

Question 2:

At certain specified conditions, A is converted to B in a reversible chemical reaction where the rate constant for forward reaction is 2 hr^{-1} and for the backward reaction is 1 hr^{-1}. In the given conditions, the product B can further convert to either C or D via two different irreversible reactions. The rate constant for B converting into C is 0.2 hr^{-1} and the rate constant for B converting into D is 0.6 hr^{-1}. A well-mixed batch reactor is used to carry out the above reactions. The feed to the reactor is a mixture of A and B with concentrations of 50 mol/L and 5 mol/L respectively. Once the feed is input to the reactor and the reactor is subject to the specified conditions, the reactions start occurring. Your team is interested to know the time at which they should open the reactor vessel and stop the reactions in order to obtain the maximum concentration of B.

From the conservation principles, write the set of equations that can assist you to resolve the above (don't attempt any analytical/numerical solution in this part). **[5 marks]**

Write a MATLAB program to solve the derived equations. **[5 marks]**

Find the optimal residence time to obtain the maximum concentration of B. **[2 marks]**

$$A \underset{1hr^{-1}}{\overset{2hr^{-1}}{\rightleftharpoons}} B \to C, \quad B \to D$$

16 0

bvp no

Question 3:

Heat transfer through a variable cross section area fin is described by the following differential equation

$$(4-5X)\frac{d^2T}{dX^2}-5\frac{dT}{dX}-2T=0$$

subject to the following boundary conditions: $T(X=0)=1$ and $\left.\frac{dT}{dX}\right|_{X=1}=0$. Here, X is the dimensionless length of fin and T is the dimensionless temperature. Using finite difference technique, convert the differential equation into a set of algebraic equations; discretization interval should not be more than 0.25. Solve the resulting set of algebraic equations in MATLAB using suitable inbuilt functions. **[10 marks]**

Question 4:

Solve the above problem using bvp4c in MATLAB. Discretization interval should not be more than 0.1. Compare the results with that of the previous scheme (Ques 3) in a single MATLAB plot. **[10+3 marks]**

Question 5:

The growth estimation of populations has many engineering and scientific applications. One of the simplest models assumes that the rate of change of the world population p is proportional to the existing population at any time t with a proportionality constant of 0.0178/yr. In year 1950 AD, the world population was 2560 million.

Implement the 4th order Runge-Kutta method in MATLAB to simulate the world population from 1950 AD to 2050 AD with a step-size of 5 years. Present the results in the form of a x-y plot (properly labelled). **[8 +2 marks]**

The actual world population in million from 1950 through 2000 was as follows:

Year	1950	1955	1960	1965	1970	1975	1980	1985	1990	1995	2000
Population (in millions)	2560	2780	3040	3350	3710	4090	4450	4850	5280	5690	6080

Calculate root mean squared error and mean absolute error between your simulated and actual population? Write a MATLAB script for your calculations. Comment on the fidelity of your simulations. **[5 marks]**

$$\frac{d^2T}{dx^2}-\frac{5}{4-5X}\frac{dT}{dx}-\frac{2}{4-5X}T=0$$

$y_1' = y_2$

$$T''-\frac{5}{4-5X}T'-\frac{2}{4-5X}T=0$$

$$y_2'-\frac{5}{4-5X}y_2-\frac{2}{4-5X}y_1=0$$