**INDIAN INSTITUTE OF TECHNOLOGY ROORKEE**

Department of Chemical Engineering

B.Tech. (ChE), End Term Examination, Autumn Semester 2024-2025

**CHN-323 Computer Applications in Chemical Engineering** **Max Marks: 65, 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. Make suitable assumptions wherever necessary.

## Question 1: [10 marks]

We wish to produce C from A and B by the following reaction network in a CSTR.

$$\begin{array}{ll} A + B \rightarrow C + D & r_{R1} = k_1(T)c_A c_B \\ C + B \rightarrow S_1 + D & r_{R2} = k_2(T)c_C c_B \\ A + D \rightarrow S_2 & r_{R3} = k_3(T)c_A c_D \\ A + B \rightarrow S_3 & r_{R4} = k_4(T)c_A c_B \\ C + B \rightarrow S_4 & r_{R5} = k_5(T)c_C c_B \end{array}$$

The volume of CSTR is 5000 L and it has an input stream with flow rate of of 1 L/s containing species A and B in a carrier solvent, such that inlet concentrations of A and B is 1 M each. The following values of rate constants are given at different temperatures.

$k_1$(298 K) = 0.01 L/(mol.s); $k_1$(310 K)= 0.02 L/(mol.s); $k_2$(T)=$k_1$(T)

$k_3$(298 K) = 0.001 L/(mol.s); $k_3$(310 K)= 0.005 L/(mol.s);

$k_3$(T) = $k_4$(T) = $k_5$(T)

You need to calculate the steady state concentration of A, B, C and D at the reactor outlet when the reactor is operated isothermally at 298 K. Write all the equations in script and then write a MATLAB program for your calculations.

## Question 2: [15 marks]

4938.298 , 0.24

Continuing with the above problem, we wish to design and operate the reactor (assumed operated isothermally) to maximize the concentration of C in the output stream. While designing, we can change the volume of the reactor V, within the range of 10 L to 10000 L. While operating the reactor, we can vary inlet concentrations of A and B and reactor temperature T. The reactor temperature can be varied in the range of 298 K and 335 K. While varying inlet concentrations of A and B, we have to make sure that the total inlet concentration of A and B is less than 2 M. Find out the optimal volume and operating conditions of CSTR.

## Question 3: [10 marks]

*Isle Royale National Park is a 210-square-mile archipelago composed of a single large island and many small islands in Lake Superior. Moose arrived around 1900, and by 1930, their population approached 3000, ravaging vegetation. In 1949, wolves crossed an ice bridge from Ontario. Since the late 1950s, the numbers of the moose and wolves have been tracked. In 1960, the populations of moose and wolves were 610 and 22. The varying populations of moose and wolves with time can be modeled using the Lotka-Volterra equations (predator-prey problem).*

$$\frac{dx}{dt} = ax - bxy$$

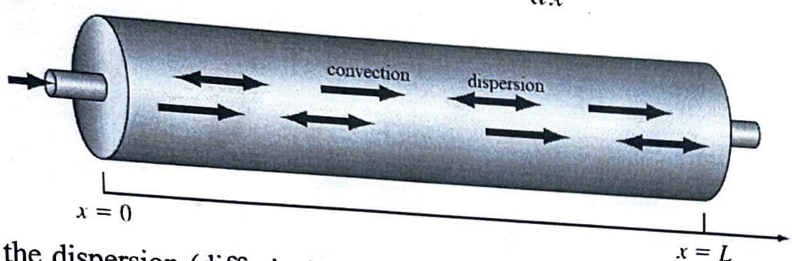
$$\frac{dy}{dt} = -cy + dxy$$

where $x$ denotes population of prey and $y$ denotes population of predator. Solve for population of both moose and wolves from 1960 to 2020 using the following coefficient values: a = 0.23, b = 0.0133, c = 0.4, and d = 0.0004. Write a program in MATLAB without using inbuilt solvers. Plot both the populations with time (on same graph) with proper axis labels and legends.

**Question 4: [20 marks]**

The following differential equation describes the steady-state concentration of a substance that reacts with first-order kinetics in an axially dispersed plug-flow reactor

$$D\frac{d^2c}{dx^2} - U\frac{dc}{dx} - kc = 0$$




where $D$ = the dispersion (diffusion) coefficient (m$^2$/hr), $c$ = concentration (mol/L), $x$ = distance (m), $U$ = the velocity (m/hr), and $k$ = the reaction rate (/hr). The boundary conditions can be formulated as

$$Uc_{\text{in}} = Uc(x=0) - D\frac{dc}{dx}(x=0)$$

$$\frac{dc}{dx}(x=L) = 0$$

where $c_{\text{in}}$ = the concentration in the inflow (mol/ L), $L$ = the length of the reactor (m). Use the finite-difference approach to solve for concentration as a function of distance given the following parameters: D = 5000 m$^2$/hr, U = 100 m/hr, k = 2/hr, L = 100 m, and $c_{\text{in}}$ = 100 mol/L. Employ finite-difference approximations with $\Delta x$ = 10 m and then write MATLAB program to obtain your solutions. ~~Compare your numerical results with the analytical solution given below by plotting them together and calculating RMSE.~~

$$c = \frac{Uc_{\text{in}}}{(U - D\lambda_1)\lambda_2 e^{\lambda_2 L} - (U - D\lambda_2)\lambda_1 e^{\lambda_1 L}} \times (\lambda_2 e^{\lambda_2 L} e^{\lambda_1 x} - \lambda_1 e^{\lambda_1 L} e^{\lambda_2 x})$$

Convective → Cu

where

Diffusive = $-D\frac{dC}{dn}$

$$\frac{\lambda_1}{\lambda_2} = \frac{U}{2D}\left(1 \pm \sqrt{1 + \frac{4kD}{U^2}}\right)$$

**Question 5: [10 marks]**

(a) Derive the differential equation given in the previous question and (b) solve it using bvp4c solver in MATLAB.

## Submission of computer codes:

Name every code with question number_your first name; put all codes in a single folder named as "your first name_roll number". Now make a zip or rar file of this folder. Email the zip file **ashwini.fch@gmail.com** and cc to **a_dharmesh@iitr.ac.in** , vidish1604@oksbi