BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI
First Semester 2022-2023
CHE G523 Mathematical Methods in Chemical Engineering
Comprehensive Examination

Date: 24.12.2022, 2-5 PM **Duration: 180 Min.** **Total Marks: 35**

CLOSED BOOK (10 Marks)

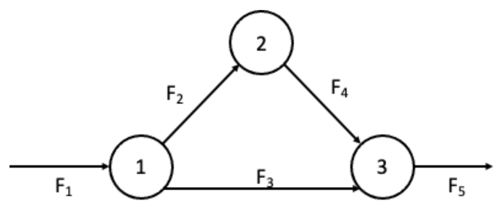
Q.1 Using the symmetric matrix $A = \begin{bmatrix} 1 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 1 \end{bmatrix}$, Compute the Eigen values.

[2 Marks]

Q.2 Write a MATLAB code to solve the ODE: $\frac{d^2T}{dx^2} + h(T_a - T) = 0$ with boundary conditions: $T(0) = T_1$ and $T(L) = T_2$.

[2 Marks]

Q.3 Consider the splitter network shown in the figure: ***F*** represents the mass flow rate. Formulate the system of vectorial form, and comment on independency and how to obtain the solution.



[2 Marks]

Q.4 Using the Finite Difference approach with explicit method, derive the recurring expression for the solution of the following PDE.

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{dx^2}$$

at $t = 0$ is 0 mol/cm^3 for all x.
for $t > 0$ C at $x = 0$ is 5 mol/cm^3.
$x = 10$ cm is $\frac{\partial C}{\partial x} = 0$.
Use a time step of 0.2 s, and 4 intervals for length coordinate. $D = 2$.

[2 Marks]

Q.5 A reversible reaction $A \leftrightarrow B$ occurs isothermally in a batch reactor. The evolution of concentrations is given by:

$$\frac{dC_A}{dt} = -C_A + 2C_B \text{ and } \frac{dC_B}{dt} = C_A - 2C_B.$$

The initial concentrations of A and B are 2 mol/cc and 3 mol/cc, respectively. Using eigenvalue method, determine the equilibrium concentration of A and B.

[2 Marks]

#All The Best#

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OPEN BOOK (25 MARKS)

Q.1 The reaction-diffusion equation for a catalyst slab in which a first-order reaction occurring is:

$$\frac{d^2C}{dx^2} = \phi^2 C$$

Where C and x are dimensionless concentration and length variables, respectively. ϕ is the Thiele modulus, which can be taken as 0.5.

The boundary conditions for the equation are: $C(0) = 0$ and $C(1) = 1$.

Solve the equation:

(A) Using the Orthogonal Collocation method, solve the governing equation for N=2.

(B) Using the Finite Difference method, solve the governing equation taking three intervals.

(C) Using the Shooting method and Euler forward method with $h = 1/3$

Tabulate *x vs C* for all three methods.

[3 × 4 Marks = 12 Marks]

Q.2 Consider the Non-Dimensional unsteady convection-diffusion heat transfer equation

$$\frac{\partial T}{\partial t} + \frac{\partial T}{\partial x} = \frac{1}{Pe}\left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right]$$

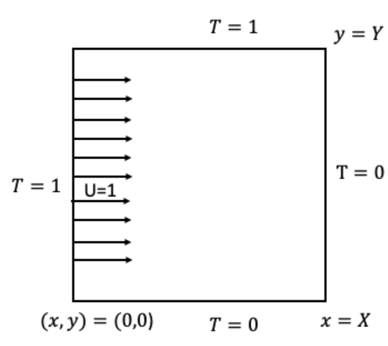
(A) Derive the finite difference upwind implicit formulation for the above PDE. Write the Gauss-Seidel formulation of the problem.

(B) Now assume steady state, we get convection-diffusion heat transfer equation as:

$$\frac{\partial T}{\partial x} = \frac{1}{Pe}\left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right]$$

(i) Derive the recurring equation with FD method with central scheme.

(ii) Solve the above equation using the finite difference method with the central scheme and $\Delta x = 1/3$, $\Delta y = 1/2$ and boundary conditions as shown in the figure and peclet number is 1.5



[4 + 9 =13 Marks]

#All The Best#