Ref. No. : Ex/ChE/T/412/2018

B.E. CHEMICAL ENGINEERING FOURTH YEAR FIRST SEMESTER – 2018

Mathematical Modeling in Chemical Engineering

Use Separate Answer-script for each part

Time: Hours

Full Marks: 100

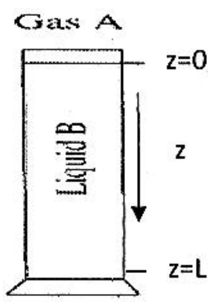
Part-I

Marks: 50

Answer question no.2 and any two from the rest

1. The stagnant liquid B in a container is exposed to reacting gas A at time t=0. The component A reacts with B while diffusing in it. The reaction is of pseudo-first order with respect to the concentration of A. The unsteady state mole balance equation of A is $\frac{\partial C_A}{\partial t} = D_{AB}\frac{\partial^2 C_A}{\partial z^2} - kC_A$ and the boundary and initial conditions are: IC: $C_A(z,0) = 0 \quad for\ z > 0$; BC 1: $C_A(0,t) = CA_0 \quad for\ t \geq 0$

BC 2: $(\frac{\partial C_A}{\partial z})_{z=L} = 0 \quad for\ t \geq 0$. Describe the algorithms for Crank Nicolson method and orthogonal collocation method to solve the partial differential equation along with the initial and boundary conditions to express the concentration of A as a function of axial length and time. **20**



(Figure 1)

Reaction:

A+B ⟶ C+D

2. For a series of reactions involving autocatalytic ones, carried out in a batch reactor, the following dynamic equations are obtained: $\frac{dX_1}{dt} = \alpha - \beta X_1 + X_1^2 X_2 - X_1$ and $\frac{dX_2}{dt} = \beta X_1 - X_1^2 X_2$ where, X_1 and X_2 represent the concentrations of components X and Y in the following reaction series: $A \rightarrow X$, $B + X \rightarrow D + Y$; $Y + 2X \rightarrow 3X$; $X \rightarrow E$. With the help of local stability analysis determine the condition which should be avoided. The concentrations of A, B, D and E are assumed constant. Locate the bifurcation point on the bifurcation diagram where X_1 is plotted as a function of parameter β,

parameter α remaining constant. Verify whether the Hopf bifurcation condition is satisfied or not. When using any method (e.g., linear stability analysis, Hopf bifurcation theorem) , state its basic principle.**10**

3. A tubular reactor of length L and unit cross sectional area is employed to carry out a 1st order chemical reaction in which A is converted to product B with a rate constant k. If the volumetric feed rate bedenoted by q and the feed concentration by C_{A0}, dispersion coefficient by D, and steady state be attained, develop the mathematical model for the system assuming the validity of Danckwerts boundary condition. Showing the information flow diagram, describe the algorithm for the suitable numerical solution of the system equation along with boundary conditions, expectedly leading to a split boundary value problem, to generate the axial concentration profile of the reactant A. 20

4. a)A solid rectangular slab at a uniform temperature T_0 has its four edges thermally insulated. The temperature of one exposed face is raised to be maintained at T_1, while the temperature of the other exposed face is held constant at T_0. Using the method of separation of variables and Sturm-Liouville Eigen value problem, solve the system equation along with boundary conditions to express temperature as a function of position and time. Sturm Liouville equation: $\frac{d}{dx}\left[p(x)\frac{dy}{dx}\right]+\left[q(x)+\lambda r(x)\right]y=0$ 10

4. b) Referring to Figure 2 showing four CSTRs in series, operated at different temperatures, and the data given in Table I , develop the system equations. Describe Gauss-Siedel algorithm to determine the steady state concentrations in 2nd, 3rd and 4th reactors.

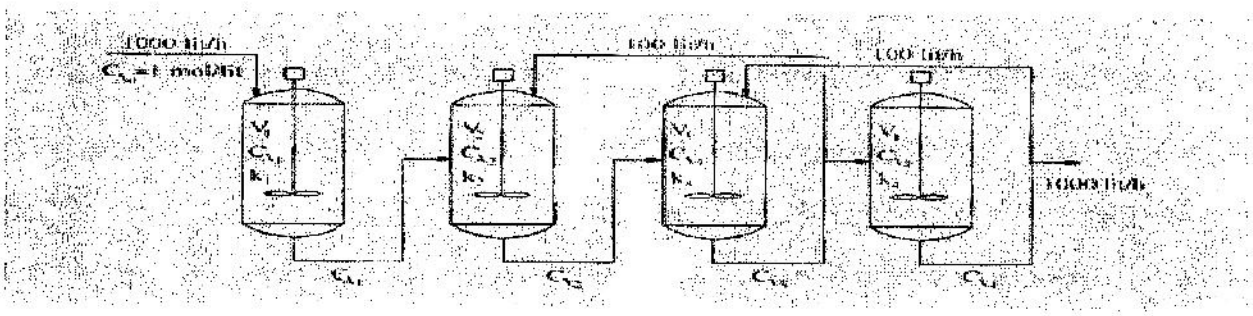


Figure 2

Table 1

Reactor	Volume (L)	Rate constant (h^{-1})
1	1000	0.1
2	1500	0.2
3	100	0.4
4	500	0.3

10

B.E. CHEMICAL ENGINEERING 4 TH YEAR 1 ST SEMESTER EXAMINATION, 2017

MATHEMATICAL MODELING IN CHEMICAL ENGINEERING

ANSWER ANY TWO QUESTIONS

ASSUME MISSING DATA, IF ANY

TOTAL MARKS:100

TIME: 3 HRS

REFERENCE NO:EX/CHE/T/412/2018

PART II

1. Use both explicit and implicit Euler methods for the adaptive ad stiff system to solve the following mathematical model:
   $dy/dt = -1000y + 3000 - 2000\,e^{-t}$
   $y(0) = 0$
   only two iterations are needed. Use appropriate value for interval of integration.
2. The following differential equation is a model for heat transfer in a long, thin rod. This is a boundary value problem.

   $d^2T/dx^2 + h(T_a - T) = 0$
   Length of the rod = 10 m
   $T_a = 20^0C$
   h = 0.01
   Boundary conditions: $T(0) = 40^0C$
   $T(L) = 200^0C$
   Formulate the finite difference approximation and present it in a matrix form. The rod is divided into four nodes excluding the boundary nodes.
3. Use implicit method to solve the following heat conduction equation. The equation is a parabolic partial differential equation.

   $k\partial^2T/\partial x^2 = \partial T/\partial t$
   $k\Delta t/\Delta x^2 = 0.020875$
   Formulate the finite difference equations considering a four node problem, The rectangular slab has temperatures of 0,50,75 and 100 degree centigrade at four different faces.
4. Use Thomas algorithm for sparse, tridiagonal matrices to solve the following problem:

$$\begin{bmatrix} 2.04 & -1 & & \\ -1 & 2.04 & -1 & \\ & -1 & 2.04 & -1 \\ & & -1 & 2.04 \end{bmatrix} \begin{bmatrix} T_1 \\ T_2 \\ T_3 \\ T_4 \end{bmatrix} = \begin{bmatrix} 40.8 \\ 0.8 \\ 0.8 \\ 0.8 \end{bmatrix}$$