Ref. No.: Ex/ChE/T/412/2018(S))

B.E. CHEMICAL ENGINEERING FOURTH YEAR FIRST SEMESTER SUPPLEMENTARY EXAM 2018

MATHEMATICAL MODELING IN CHEMICAL ENGINEERING

Time: 3 hours **Total Marks:100**

Answer any four questions.

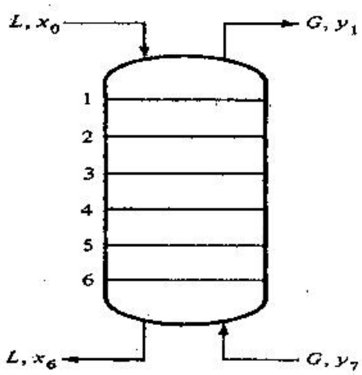
Use graph paper if required. Assume any missing data.

All symbols have usual significance

1. It is desired to develop the steady state tray composition for a steady state tray composition for a 6-plate absorption column. It can be assumed that the linear equilibrium relationship between liquid and gas phases on each plate:

$$y_m = ax_m + b$$

The inlet composition to the column x_0 and y_7 are specified along with the liquid (L) and gas (G) phase flow rates (moles/time). The system is shown schematically in Figure 1:



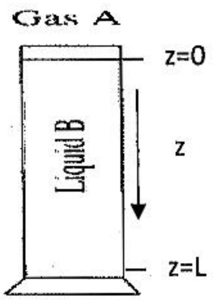
Typical values of parameters are as follows: a = 0.72; b=0; G = 66.7kmol/min and L= 40.8 kmol/min. Write down the steady state lumped model equations by making material balance and describe the algorithm for the suitable numerical method for solution. 25

2. 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. 25

3. 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. **25**



(Figure 1)

Reaction:

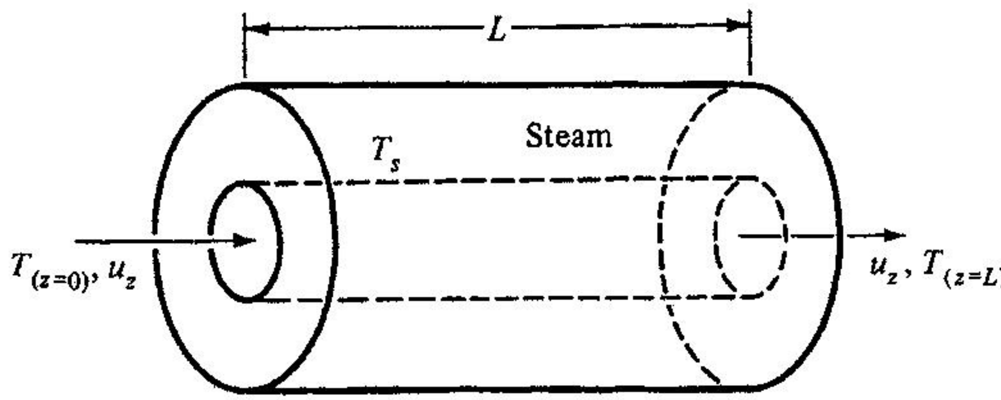
A+B ⟶ C+D

Reaction rate constant = k

4. a)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 $\frac{dX_1}{dt} = \beta X_1 - X_1^2 X_2$ where, X_1 and X_2 represent the concentrations of components X and Y in the following reaction series: $A \to X$, $B + X \to D + Y$; $Y + 2X \to 3X$; $X \to E$. 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. 15

4. b) State the principles of orthogonal collocation method with reference to obtain the solution of unsteady state mole balance equation of problem No. 2. 10

5. It is intended to develop the dynamic response of a steam heated plug flow heat exchanger.



The dynamic response of the axial temperature profile of the fluid flowing in the inner tube for a step change in the inlet temperature ($T_{(z=0)}$) is to be computed. Temperature of steam, T_s, is constant. The energy balance equation around the tube is as follows:

$$\frac{\partial T}{\partial t} = -v_z \frac{\partial T}{\partial z} + \frac{4U}{\rho c_p D}(T^s - T)$$

For this problem,

B.C 1: T(z) at t=0 is a known steady state profile

B.C. 2 T at z=0 (t>0) is T_0. Describe the method for solution. 25

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