B. Tech. (Chemical Engineering) Eighth Semester (C.B.S.)

Computational Chemical Engineering Paper - I

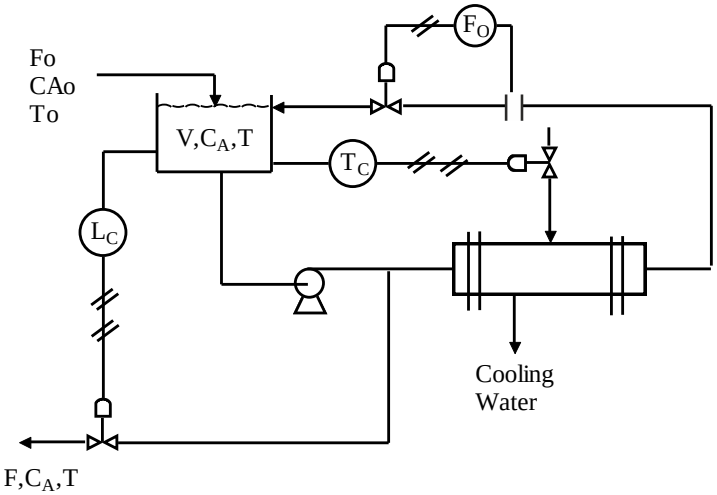
P. Pages : 2 **TKN/KS/16/7844**

Time : Three Hours * 0 4 0 2 * Max. Marks : 80

Notes : 1. All questions carry equal marks.
2. Answer **any five** questions.
3. Assume suitable data wherever necessary.

1. When cooling jacket and internal cooling coils do not give enough heat transfer area, a circulating cooling system is sometimes used. Process fluid from the reactor is pumped through an external heat exchanger and back into the reactor. Cooling water is added to the shell side of the heat exchanger at a rate F_W as set by temperature controller. The circulation rate through the heat exchanger is constant. Assume that the shell side of the exchanger can be represented by two perfectly mixed 'lumps' in series and that the process fluid flows counter current to the water flow, also through two perfectly mixed stages. The reaction is irreversible and first order in reactant $A : A \xrightarrow{k} B$. **16**

The contents of the tank are perfectly mixed. Neglect reactor and heat exchanger metal. Derive a dynamic mathematical model of this system.



2. A reversible reaction $2A + B \leftrightarrows C$ can be characterized by the equilibrium relationship $k = \dfrac{C_c}{C_a^{\,2}\, C_b}$ Suppose that we define a variable x as representing the number of moles of C that are produced. Conservation of mass can be used to reformulate the equilibrium relationship as $k = \dfrac{(C_{co} + x)}{(C_{ao} - 2x)^2 (C_{bo} - x)}$ where the subscript 0 designates the initial concentration of each constituent. If k = 0.015, $C_{ao} = 42$, $C_{bo} = 30$ and $C_{co} = 4$, compute x using suitable numerical method. **16**

3. In a certain heat transfer process the following equations appear: **16**

$$80T_1 - 15T_2 + 7T_3 - 5T_4 = 700$$
$$10T_1 - 60T_2 + 4T_3 - 9T_4 = -1300$$
$$8.5T_1 - 2.3T_2 + 45T_3 - 10T_4 = 1000$$
$$2.6T_1 - 7.2T_2 + 3.2T_3 - 40T_4 = -1800$$

obtain T_1, T_2, T_3 and T_4 by Gauss-Seidal method. Calculate the approximate relative error in each iteration. Report the results in tabular form.

4. a) The specific volume of a superheated steam is listed in steam tables for various temperatures. For example at a pressure of $2950\,lb/m^2$, absolute; we have following data **10**

T(°F)	700	720	740	760	780
ν	0.1058	0.1280	0.1462	0.1603	0.1703

Determine ν at T=750 °F.

b) Discuss the criteria for a "Best" fit. **6**

5. The following equations define the concentrations of three reactants **16**

$$\frac{dc_1}{dt} = +\,20c_1 c_3 - 2c_2$$

$$\frac{dc_2}{dt} = 20c_1 c_3 - 2c_3$$

$$\frac{dc_3}{dt} = +\,20c_1 c_3 - 2c_3 - 0.2c_2$$

If initial conditions are $c_1 = 500$, $c_2 = 0$ and $c_3 = 500$, Find the concentrations for the times from 0 to 30 sec.

6. Use the implicit method to solve for the temperature distribution of a long, thin rod with a length of 10cm and the following values **16**

$k^1 = 0.49\,cal/(5\cdot cm\cdot{}^\circ C)$

$\Delta x = 2cm$

$\Delta t = 0.1sec$

At t = 0, the temperature of the rod is zero and the boundary conditions are fixed for all times at T(0) = 100°C and T (10) = 50°C. Note that the rod is aluminum with

$C_P = 0.2174\,Cal/9^\circ C$ and $\rho = 2.7\ 9/cm^3$

Take $k = \dfrac{k^1}{\rho C_P}$

$$\lambda = \frac{k\Delta t}{(\Delta x)^2}$$

7. a) Explain the principles of formulation of mathematical model. **8**

b) Develop mathematical model for isothermal CSTR in which following reaction takes place $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ state your assumptions. **8**

8. Develop mathematical model for Non-ideal distillation column. State your assumptions clearly. **16**

****