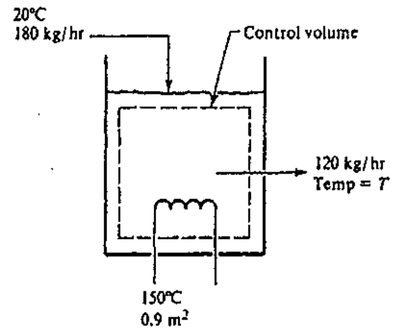
Ref. No. Ex/ChE/PC/B/T/325/2025

B.E. CHEMICAL ENGINEERING 3rd YEAR SECOND SEMESTER EXAMINATION, 2025

SUBJECT: MATHEMATICAL MODELLING IN CHEMICAL ENGINEERING
Time: 3 hours **Full Marks (100)**

Q.No.	CO	State all the assumptions. Assume missing data (if any). Answer all the questions	Marks
1.(i)	1	**Compare between lumped parameter model and distributed parameter model. Give an example of each model.**	(2+2)
		 FIG.1	
1.(ii)	2	**A dilute solution at 20°C is added to a well-stirred tank at the rate of 180 kg/hr. A heating coil having an area of 0.9 m^2 is locate-d in the tank and contains steam condensing at 150oC. The heated liquid leaves at 120 kg/hr and at the temperature of the solution in the tank. There is 500 kg of solution at 40°C in the tank at the start of the operation. The over-all heat transfer coefficient is 342 kcal/hr m2 °C and the heat capacity of water is 1 kcal/kg°C. Write the model equations and draw the information flow diagram. Calculate the outlet temperature after 1 hr. Refer to Fig.1**	(3+3+2)
2. (i)	2,4	**Consider single-stage multi-component isothermal flash distillation. Draw the schematic of the process and define the variables. The feed temperature, composition, equilibrium temperature and pressure are known. Write the generalized model equations. For composition independent equilibrium constant K values, simplify the model equations for the simulation of percent vaporization (ψ), liquid and gas phase composition. Draw the information flow diagram for isothermal flash and write the algorithm of the numerical technique to be used for solving the percent vaporization (ψ).**	(5+5)
(ii)		**A 100 kmol/h feed consisting of 10,20,30,40 mol% of Propane, n-Butane, n Pentane and n Hexane, respectively is isothermally flash distilled at a constant pressure and temperature. At a flash temperature 366.5 K and 689.5 kPa the Ki values (independent of composition) for Propane, n Butane, n Pentane and n Hexane are 4.2, 1.75, 0.74 and 0.34, respectively. Calculate the percent vaporization and liquid and vapor phase compositions using the algorithm in question (iii). (show the iteration wise results and convergence.**	(10)

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Q.No.	CO	State all the assumptions. Assume missing data (if any). Answer all the questions	Marks
3.	2,4	**A continuous stirred tank chemical reactor where a single second order reaction occurs. The inlet flowrate is F_{in} litter/min and the outlet flowrate F is a function of liquid height ($F=\beta h^{1/2}$) in the tank. Write the dynamic model equations. Calculate the steady state concentration Cs of the reactant A and the height of the liquid (hs) in the reactor for the following values of input variables and parameters: Fin=1 liter/min, Cin=1 gmol/liter, A (cross-sectional area of the reactor)=1m^2, k=2 liter/(gmol min), β=1 liter/ (min m$^{1/2}$). Linearize the model equations around the steady state and express the dynamic equations in state-space form. Find the stability of the steady state. What kind of Phase plot do you expect?**	(4+2+5+4+3)
4.	3,4	**Consider an isothermal tubular reactor with axial mixing (TRAM) with irreversible 1st order chemical reaction ($r_A=-kC_A$).**	
		(i) Write the steady state species balance equation. Use Dankwert's boundary condition at the inlet. Non-dimensionalize the model equation and boundary conditions.	(4+4)
		(ii) Draw an IFD for solving the above problem using shooting method.	(3)
		(iii) Consider the finite difference technique to solve the BVP. Discretize the equation and derive the form of the matrix. What is the form of the matrix? Write the name of the algorithm to solve dimensionless concentration at different grid points.	(5+2+2)
5	2,4	**Consider a constant volume non-isothermal CSTR with jacket cooling where reactant A is converted to product by a first order reaction ($A \longrightarrow B$). (i)Write the dynamic model equations (overall material balance, component balance and energy balance). For the parameter set given below 350 K and 0.5 gmmole /lit are the steady state temperature and concentration.(ii)Linearize the model equations around the steady state and express the dynamic equation in state-space form. Check the stability of the steady state. What kind of phase plot do you expect? Data: F (feed rate)= 100 liters/min, V(volume)=100 liters, Tj(jacket temperature)=300K, ko(reaction rate constant)=7.2x10^{10}min^{-1}, ($-\Delta H$) (Heat of reaction)=50000 J/gm mole, E/R =8750 K, ρC_p=239 J/liter K, T_f(feed temperature)=350 K, C_{Af}(feed concentration)=10 kgmole/m^3, UA= 50000 J/min K**	(5+5+3+2)
	5	**(iii) Derive a single nonlinear algebraic equation ($F(x,\mu)=0$) by equating the rate of heat generation and rate of heat removal from a non-isothermal CSTR at steady state and substituting the steady state concentration (C_{As}) in terms of steady state temperature Ts. (μ is a parameter set those can be varied). Discuss about multiple steady state. Write the mathematical conditions of bifurcation. Check whether the conditions for Saddle node bifurcation (function and its first derivative zero but 2nd derivative is non zero) is valid in this specific case.**	(4+5+2+4)