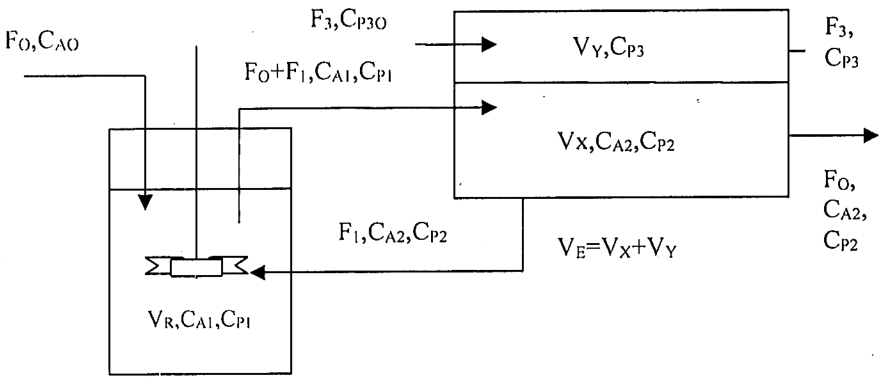
Ref. No. : Ex/PG/ChE/T/128C/2024

M. CHEMICAL ENGINEERING FIRST YEAR SECOND SEMESTER EXAMINATION 2024
SUBJECT: MODELLING AND SIMULATION OF CHEMICAL PROCESSES

Time: Three hours Full Marks 100

No. of Questions	Answer Question 1(a) or 1(b), any two from questions 2(a) 2(b),2(c), and the rest.	Marks
1(a)	 Fig.1 Integrated reactor and liquid -liquid extractor Often it is necessary to extract a product, which impedes a reaction in a CSTR. This is accomplished with an integrated liquid-liquid extraction unit (refer to Fig. 1). Consider a CSTR with reaction $A \longrightarrow P$ The kinetics exhibit inhibition by the product: $-r_A=r_p=k_1C_A/[1+C_p/K_I]$, where k_1 is the reaction constant and K_I is the inhibition constant. Develop the transient model equations for the CSTR and integrated extractor. Identify the state variable matrix, input variable matric and function matrix. OR	(10)
(b)	Consider a constant volume non-isothermal batch reactor where a first order exothermic elementary reaction $A \longrightarrow P$ occurs. The temperature of the reactor is controlled by manipulating the cooling water flowrate through a jacket. Write the model equations and draw the information flow diagram.	(10)

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2.(a)	Consider single-stage multi-component isothermal flash distillation. Draw 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).	(10) (5+5)
2(b)	Consider a multicomponent distillation column having 3 equilibrium stages, a partial condenser, a partial reboiler. The saturated liquid feed consisting of 3 components is introduced at the middle plate. (i)Write the MESH equations of conservation of mass (M), energy (H) and of equilibrium (E) (for the above specific case). (ii) You need to solve the above equations using Bubble Point method. Draw the algorithm (flowchart).	(8) (12)
2(c)	Consider a batch polymerization reactor where the monomer (example Styrene) is polymerized by free radical (chain growth) mechanism. Write the kinetic expression of initiation, propagation and termination through combination and disproportioanation. Write the model equations. Define the zeroth and first moment of polymer radical and dead polymer. Derive an expression for rate of monomer conversion considering QSSA for transient species.	(8+2+10)
3.	Consider a non-isothermal CSTR with jacket cooling where reactant A is converted to product by a first order reaction (A $\longrightarrow$ B). Assume constant volume system and constant density system. Write the dynamic model equations. Linearize the model equations around the steady state and express the dynamic equation in state-space form (in terms of deviation variables) and check the stability of the steady state C_{As}=5.518, T_s=339.1, for the following set of parameters and input variable data. Data: F/V, hr-1=1, Ko hr-1 = 9703*3600; (-ΔH) Kcal/kgmol = 5960; E, kcal/kgmol = 11843; ρCp kcal/m^3 °C= 500; T_f °C=25; C_{Af} kgmol/m^3= 10 ;UA/V kcal/m3°C hr=150; T_j °C= 25. What kind of Phase plot do you expect? Show the phase diagram.	(4+4+4+4)
	Derive a single steady state energy balance equation G(Ts, μ) = 0 (by Qgen-Qr=0) where Ts is the state variable and μ is the vector of physical parameters that can be varied. Discuss about multiple steady state behavior and cusp catastrophe.	(3+6)

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No. of Questions	Answer Question 1(a) or 1(b), any two from questions 2(a) 2(b),2(c), and the rest.	Marks
4.	A tubular chemical reactor (plug flow reactor with axial dispersion) of length L and cross section 1 cm^2 is employed to carry out a first order chemical reaction in which material A is converted to product B : A $\longrightarrow$ B. The specific rate constant is k s^{-1}. Feed rate is u m^3/s and feed concentration is C_o mol m^{-3} and axial diffusivity is assumed to be constant D m^2/s. Assume that there is no volume change during the reaction and steady state conditions are established. Consider an entry length preceding the reactor section where no reaction occurs	
	(i) Derive the model equation for concentration of solute as a function (z) of axial position. Use Dankwert's boundary condition at the inlet. Nondimensionalize the equations and boundary conditions and obtain the dimensionless numbers.	(7)
	(ii) Draw the information flow diagram to solve for the dimensionless concentration. Discuss about shooting method.	(4+4)
	(iii) For numerical solution use finite difference method. Discretize the governing equation and insert the boundary conditions to derive the matrix equation. What kind of matrix would you get? Name the numerical algorithm to solve the same.	(10)