M. CHEMICAL ENGINEERING FIRST YEAR SECOND SEMESTER SUPPLEMENTARY EXAMINATION 2025

SUBJECT: MODELLING AND SIMULATION OF CHEMICAL PROCESSES

Time: Three hours Full Marks 100

State all the assumptions. Assume any missing data.

No. of Questions	Answer any 2 questions from question 1-3 and all the rest.	Marks
1.	Consider a plate type 5^{th} stage (counter current) absorption column. The liquid feed (entering at the top plate) flow rate L=100 kgmole inert oil/hr, gas feed (entering at the bottom plate) flow rate V =120 kgmole air/hr, liquid feed composition xf=0.0 kgmole Benzene/kgmole inert oil, gas feed composition y6=0.25 kgmol Benzene/kgmole air. Assume that liquid molar hold up for each stage is M =6 kgmol. Assume a linear equilibrium relationship yi=axi ; a=0.5. Write the steady state model equations for any intermediate stage i, for top stage and bottom stage. Derive the steady state matrix equations for plate composition (x_i). Name the numerical technique for solution of steady state plate-composition-	(15)
2.	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. (ii) You need to solve the MESH equations using Bubble Point method. Draw the algorithm (flowchart).	(15)
3.	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. (ii)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	
4.	Consider a process that uses bacteria to produce antibiotic. The reactor is contaminated with protozoan that consumes bacteria. Assume that predator – prey equations are used to model the system (x1 : bacteria (prey), x2 : protozoa (predator). The time unit is in days. $\frac{dx1}{dt} = \alpha x1 - \gamma x1\, x2\,;\ \frac{dx2}{dt} = \varepsilon\gamma x1 x2 - \beta\, x2$ (i)What are the trivial and nontrivial steady state concentration x1s, x2s? (ii)Use the nontrivial steady state values of x1 and x2 to scale the variables as y1=x1/x1s and y2=x2/x2s and derive the governing equations in terms of scaled variables y1 and y2.	(2+2) (6)

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	(iii)Linearize the scaled equations and write in state space form. Find the eigen values of the Jacobian around the nontrivial steady state (i.e $y1s=1$, $y2s=1$) in terms of α and β. Evaluate the eigen values for $\alpha = \beta=1$. Discuss about the stability of the nontrivial steady state. What type of phase plane plot (y1 vs y2) do you expect?	(6+4)
5.	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 (overall material balance, component balance and energy balance). Linearize the model equations around the steady state and express the dynamic equation in state-space form (in terms of deviation variables). 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.	(15)
	Data:F/V, hr-1=1, Ko hr-1 = 9703*3600; ($-\Delta H$) 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.	
	Derive a single steady state energy balance equation $G(Ts, \mu) = 0$ (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 behaviour and cusp catastrophe.	(15)
	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. 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. Derive the differential model equation for concentration of solute as a function (z) axial position. Nondimensionalize the equations and boundary conditions and obtain the dimensionless numbers. For numerical solution discretize the governing equation by Finite difference method and insert the boundary conditions to derive the matrix equation. What kind of matrix would you get? Mention the numerical algorithm to solve the same.	(10+10)