Ref. No. Ex/ChE/PC/B/T/325/2024

B. E. CHEMICAL ENGINEERING 3rd Year SECOND SEMESTER EXAMINATION, 2024

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

Q.No. 1. — CO 1 — Marks 6x1= 6

Match the following

Group A	Group B
(i) Tubular reactor	(i)Discrete model
(ii) Ideal CSTR	(ii)Continuous model
(iii) Tray column absorber	(iii)Lumped parameter model
(iv) Path of a tornado	(iv)Distributed parameter model
(v) Packed bed absorber	(v)Population balance model
(vi) Molecular weight distribution	(vi) Stochastic model

Q.No. 2.(i) — CO 2 — Marks 6; 5+5+2

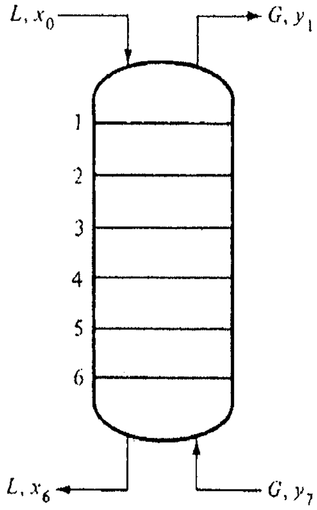

Plate type Absorption column

Consider a plate type 6th 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 G =120 kgmole air/hr, liquid feed composition xf=0.0 kgmole Benzene/kgmole inert oil, gas feed composition y7=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.

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Time: 3 hours **Full Marks (100)**

Q.No.	CO	State all the assumptions. Assume missing data (if any). Answer all the questions	Marks
2(ii)	2	Consider the batch distillation of Benzene, Toluene and Xylene in a vessel holding Mo kgmole (liquid) and a heating rate of Q Kcal/hr. At t=0 the initial compositions of Benzene, Toluene and Xylene are known. Write the model equations and draw the information flow diagram (IFD) for solving moles, compositions and temperature of the liquid in the vessel as a function of time.	(5+5)
3(i)	2,4	Consider a non-isothermal CSTR with jacket cooling where reactant A is converted to product by a first order reaction ($A \rightarrow B$). 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. What kind of Phase plot do you expect? 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.	(5+5+5)
3(ii)	2,5	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 behaviour and cusp catastrophe.	(5+4+4)
4.	2,4	Consider a batch polymerization reactor where free radical (chain growth) polymerization of Styrene occurs. By what mechanism the population (number density) of Polymer radical and dead polymer of chain-length 'n' is varied in such a reactive system? Write the kinetic expression of initiation, propagation and termination through combination and disproportioanation. Define the 1st moment of Polymer radicals and dead polymers. Write the model equations. Derive an expression for rate of monomer conversion considering QSSA for transient species.	(20)
5.		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 : $A \rightarrow B$. The specific rate constant is k s^{-1}. Feed rate is u m^3/s and feed concentration is C_0 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	
	3 3	(i)Derive the differential 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.	(6) (3)
	4 4	(ii)Draw the information flow diagram to solve for the dimensionless concentration. (iii) Discuss about shooting method for solving the problem. Write the algorithm, (iv) 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.	(5) (10)