Ref. No. Ex/ChE/PC/B/T/325/2022

B. CHEMICAL ENGINEERING 3rd YEAR SECOND SEMESTER EXAMINATION, 2021-22

SUBJECT: MATHEMATICAL MODELLING IN CHEMICAL ENGINEERING

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

Use Separate Answer Scripts for Part I and Part II

PART I (50 Marks)

State all the assumptions. Assume missing data (if any)

Q.No.	CO No		Marks
1(i)	1	Differentiate between lumped parameter model and distributed parameter model	(2)
(ii)	1	Consider batch 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' can be varied in such a reactive system? Define zeroth moment and 1st moment of Polymer radicals and dead polymers.	(4)
1(iii)	5	Show that the following system exhibits a pitchfork bifurcation with three real solutions (one stable, two unstable) for $\mu<0$ and a single unstable real solution for $\mu>0$ $$\frac{dx}{dt} = f(x, \mu)=\mu x+x^3$$	(4)
2.		A feed F to the flash tank is split into a vapor product V and a liquid product L. The feed contains NC number of components. The temperature and pressure are maintained constant. A heat exchanger keeps constant temperature and a valve on the vapor product stream that keeps constant pressure. Assume ideal liquid mixture and ideal gas (Raoult's law).	
	2	(i)Write the material and component balance equations. For composition independent equilibrium constant K values, simplify the model equations for the simulation of percent vaporization (ψ), liquid and gas phase composition.	(4)
	2	(ii)Draw the information flow diagram and write the algorithm of the numerical technique to be used for solving the percent vaporization (ψ).	(4)
	4	(iii) A 100 kmol/h feed consisting of 20,15,35,30 mol% of Propane, n-butane, n pentane and n hexane, respectively is isothermally flash distilled at a constant pressure 689.5 kPa and 367 K temperature. At this flash temperature and pressure 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, liquid and vapor phase composition.	(4)

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3.		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	
	3	(i) Derive the differential model equation for concentration of solute as a a function (z) axial position. Use Dankwert's boundary condition at the inlet.	3
	3	(ii) Nondimensionalize the equations and boundary conditions and obtain the dimensionless numbers.	3
	4	(iii) Draw the information flow diagram to solve for the dimensionless concentration. Discuss about shooting method.	3
	4	(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.	4
4.		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.	
	4	(i) Write the dynamic model equations (overall material balance, component balance and energy balance). For the parameter set given below show that 350 K and 0.5 gmmole /lit are the steady state temperature and concentration.	(5)
	4	(ii) Linearize the model equations around the steady state and express the dynamic equation in state-space form (in terms of deviation variables). Evaluate the eigen values and check the stability of the steady state. What type of phase plot do you expect?	(5)
		Data: F (feed rate)= 100 liters/min, V(volume)=100 liters, Tj(jacket temperature)=300K, ko(reaction rate constant)=$7.2 \times 10^{10} min^{-1}$, ($-\Delta H$) (Heat of reaction)=50000 J/gm mole, E/R =8750 K, ρCp=239 J/liter K, T_f(feed temperature)=350 K, C_{Af}(feed concentration)=10 kgmole/m^3, UA= 50000 J/min K	
	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.	(5)

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B.E. CHEMICAL ENGINEERING THIRD YEAR SECOND SEMESTER - 2022

3rd Year, 2nd Semester

MATHEMATICAL MODELLING IN CHEMICAL ENGINEERING

Use Separate Answer Scripts for Part I and Part II

Time: 3 Hours | Full Marks: 100

PART II (50 Marks)

Answer Q1 any One from the rest.

Q1. **[3+12+15=30]**

a) Explain a Sturm-Liouville problem.

b) Expand the function $f(x) = e^x$ in terms of the eigenfunctions of the Sturm-Liouville problem $y'' + \lambda y = 0$ (1) with boundary conditions: $y'(0) = 0$ (2); and $y(\pi) = 0$ (3).

c) Consider a diffusive-reactive system of a species B, which gets produced when A reacts. $A \rightarrow B$ is an elementary first order reaction with specific rate constant for production of B being k_B. Using the eigenfunctions of

$$C_B'' + k_B \cdot C_B = 0 \quad (1)$$

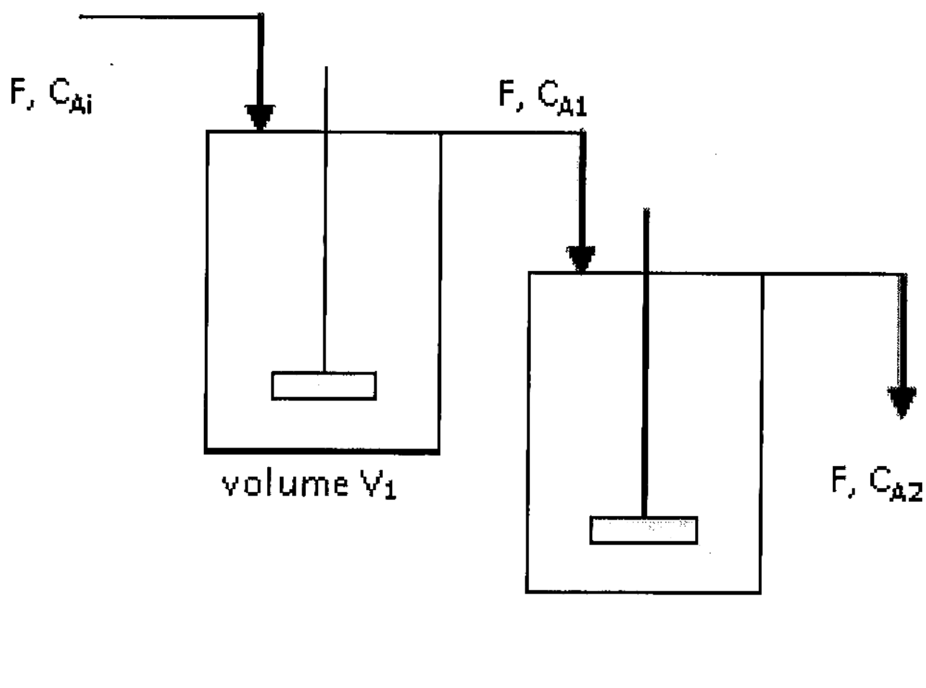
$$C_B(0) = 0 \quad (2)$$

$$C_B'(1) = 0 \quad (3)$$

expand the function $C_B(x) = 1$.

Q2. **[20]**

Consider two tanks in series with single inlet and outlet streams as shown in the following representative sketch. Starting with the component material balance for the reactant A for each of the tanks, develop a mathematical model for the continuous blending tanks in series. Solve the coupled linear Ordinary Differential Equations [ODEs] that represent the concentration in each tank, using Laplace Transforms and any other specific Operational Transforms.



Q3. **[20]**

Consider a steady-state 2-D diffusion of carbon monoxide from a square area source in a forest after an episode of a forest-fire. *Neglect any further generation or depletion through atmospheric chemistry-based routes.*

(i) Reduce the species continuity equation into an elliptic PDE of the form of a Laplace's equation. Show the steps to solve this using finite differences.
(ii) Generate the recursion formula using uniform grids in x and y directions.
(iii) Consider a case where the square has sides of length L, and the boundary conditions are such that the concentration is fixed at 20 on the left, right, and bottom sides, and fixed at 0 on the top. Discretize the domain in each direction suitably.