

B.E. CHEMICAL ENGINEERING SUPPLEMENTARY EXAMINATION 2023
 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 I

Answer any Two from Q1, Q2 and Q5 and any One from Q3 and Q4

Q1. Fourier Transforms and Its Applications**[5+15= 20]**

- a) Define Fourier Transform.
- b) Solve the following one-dimensional mass diffusion equation under unsteady state condition using Fourier transform:

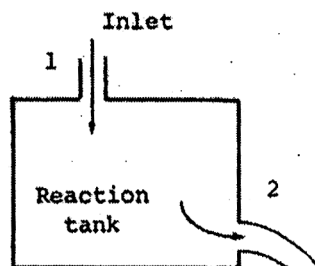
$$\frac{\partial C}{\partial t} = K \frac{\partial^2 C}{\partial x^2}$$

Q2. Develop a Population Balance Model for bacterial cell growth in a Fed Batch Fermenter.**[20]****Q3.****[3+7=10]**

- a) Distinguish between discrete and continuous variables w.r.t definition and model.
- b) Brine containing 25% salt by mass flows into a well- stirred tank at a rate of 26 kg/min. The tank initially contains 900 kg of brine containing 12% salt by mass, and the resulting solution leaves the tank at a rate of 12 kg/min. Find an expression for the amount of salt in terms of time θ .

Q4.

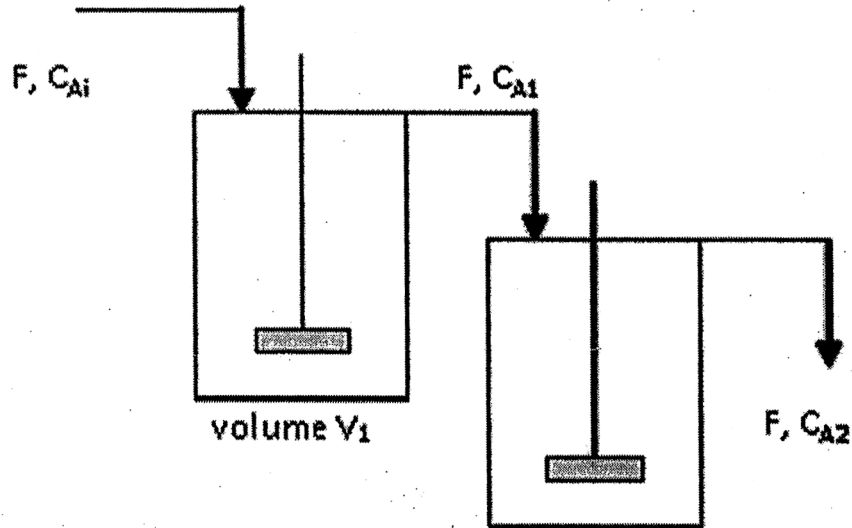
A well-stirred tank of 100 ft³ volume initially contains 5 lbm/ft³ of a substance A in a liquid form. An inlet stream with 15 lbm/ft³ of A flows into the tank at a rate of 10 ft³/rain. If the reaction $A \rightarrow C$ is a constant volume, steady flow process, how does the concentration of A in the tank vary with time? Assume the generation of A in lbm/ft³ sec. can be expressed as $v_A = -k p_A$ with $k = 0.1/\text{min}$.

[10]**Q5.****[20]**

- a) 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

[Turn over

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.



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PART-II		
Question/CO		Marks
1(i)/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 1 st moment of Polymer radicals and dead polymers.	(6)
1(ii)/1	Define lumped parameter model and distributed parameter model. Give an example of each model.	(4)
2(i)/2	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 $x_f=0.0$ kgmole Benzene/kgmole inert oil, gas feed composition $y_6=0.25$ kgmol Benzene/kgmole air. Assume that liquid molar hold up for each stage is M =6 kgmol. Assume a linear equilibrium relationship $y_i=ax_i$; $a=0.5$. 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).	(8)
2(ii)/4	Name the numerical technique for solution of steady state plate-composition-	(2)
3(i)/2	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 (x_1 : bacteria (prey), x_2 : protozoa (predator). The time unit is in days. $\frac{dx_1}{dt} = \alpha x_1 - \gamma x_1 x_2; \frac{dx_2}{dt} = \epsilon \gamma x_1 x_2 - \beta x_2$	
3(ii)/2	(i)What are the trivial and nontrivial steady state concentration x_{1s} , x_{2s} ?	(2)
	(ii)Use the nontrivial steady state values of x_1 and x_2 to scale the variables as $y_1=x_1/x_{1s}$ and $y_2=x_2/x_{2s}$ and derive the governing equations in terms of scaled variables y_1 and y_2 .	(3)
3(iii)/4	(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 $y_{1s}=1$, $y_{2s}=1$) 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 (y_1 vs y_2) do you expect?	(5+4+3)

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Answer all the questions			
Question/CO			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 $k \text{ s}^{-1}$. Feed rate is $u \text{ m}^3/\text{s}$ and feed concentration is $C_0 \text{ mol m}^{-3}$ and axial diffusivity is assumed to be constant $D \text{ m}^2/\text{s}$. 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	
4(i)	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.	(3)
4(ii)	3	(ii) Nondimensionalize the equations and boundary conditions and obtain the dimensionless numbers.	(3)
4(iii)	3	(iii) Draw the information flow diagram to solve for the dimensionless concentration. Discuss about shooting method.	(3)
4(iv)	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)