Code No: 07A70804 **R07** **Set No. 2**

IV B.Tech I Semester Examinations,May 2011
PROCESS MODELING AND SIMULATION
Chemical Engineering

Time: 3 hours **Max Marks: 80**

Answer any FIVE Questions
All Questions carry equal marks

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1. (a) Fluid is flowing through a Constant - diameter cylindrical pipe. Assume flow is turbulent, plug flow. No radial gradients exist in velocity or any other properties. Write down the total continuity equation for the system. Density and velocity are functions of both t and z.
   (b) Write down component continuity equations for the above system if a first order simultaneous reactions is taking place inside the pipe. [8+8]

2. Explain the procedure to find the bubble point temperature (BUBL T) of a binary vapour-liquid mixture. Explain the algorithm by block diagram. [16]

3. Write the model equations involved in a Batch reactor when it is in the heating phase. [16]

4. Describe the simulation of Batch reactor using Euler's Method. [16]

5. An irreversible exothermic reaction $A \xrightarrow{K_1} B$ occurs in a series of three perfectly mixed CSTRs as shown in figure 1. Feed enters the first reactor and product leaves the third reactor. Assume the reaction is n^{th} order in reactant A. Derive the mass balance and component continuity equations considering variable holdups. Assume constant density for the system, which is a binary mixture of A and B. [16]

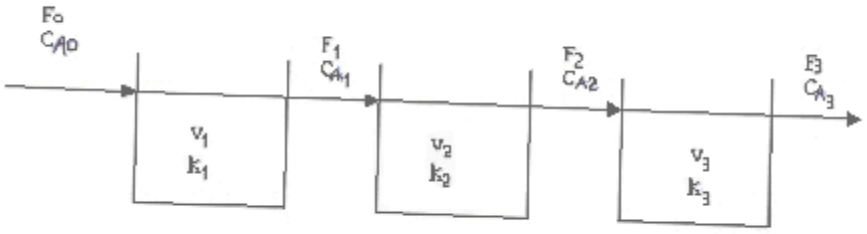

Figure 1:

6. Thermal conductivity' of the metal strip was measured at various time intervals during the heating and the values are given in the following table:

Time. t (mm)	1	2	3	4	5	6
Temp., T(^{0}C)	70	83	100	124	152	190

If the relationship between the temperature. T and time, t is of the form $T = be^{t/4} + a$, estimate the coefficients (a and b) using least square regression technique and estimate the temperature at t = 8 min. [16]

7. Find the roots of the following function $f(x) = (2x-5)^4 - (x^2-1)^3$, using false position method. [16]

8. Consider the following ODE Solve this ODE Using Runge-Kutta 4th Order Method. $\frac{dy}{dx} = 4y - e^{-x}, \quad y_0 = 1.0, \quad \Delta x = 0.1..$ [16]

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Code No: 07A70804 **R07** **Set No. 4**

IV B.Tech I Semester Examinations,May 2011
PROCESS MODELING AND SIMULATION
Chemical Engineering

Time: 3 hours **Max Marks: 80**

Answer any FIVE Questions
All Questions carry equal marks

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1. Compare approximate values of 'p' at L=0.1 and L=0.2 for differential equation $\frac{dp}{dL} = p + L^2$, with p = 1 at L=0 using Euler's Method [16]

2. An irreversible exothermic reaction is carried out in a single perfectly mixed non-isothermal CSTR. The reaction is $A \xrightarrow{K_1} B$. The reaction is nth order in reactant A and has heat of reaction 'λ' (energy units/mole of A reacted). Negligible heat losses and constant densities are assumed. To remove the heat of reaction, a cooling jacket surrounds the reactor. Cooling water is added to the jacket at a constant volumetric flow rate. Develop a mathematical model for the system considering cooling jacket as lumped one. State all the assumptions made and explain the notations scheme used clearly. [16]

3. Write the component continuity equations for a perfectly mixed batch reactor (no inflow or outflow) with first-order isothermal reactions.
   (a) Consecutive.
   (b) Reversible. [16]

4. Draw an analog computer simulation circuit diagram for solving the model equations of three ideal CSTR's in series (open loop). [16]

5. (a) Illustrate "Mass-transfer Limited" and "Chemical-rate Limited reactors" phenomena's with an example.
   (b) Derive the model equations involved in the "reactor with mass transfer". [6+10]

6. Develop a mathematical model for a simple gravity flow tank into which an incompressible liquid is pumped at a variable flow rate of F_0 (m^3/s). This inflow rate can vary with time because of changes in operations upstream The height of the liquid in the vertical cylindrical tank is h (m). The flow rate out of the tank is F (m^3/s). Discuss the Newton-Raphson algorithm for solving the modeled equations. [16]

7. At room temperature sucrose is hydrolyzed by the catalytic a action of the enzyme invertage as follows Sucrose $\xrightarrow{\text{Invertage}}$ Product. Starting with a sucrose concentration C_{AO} = 1.0 millimol/lit and an enzyme concentration C_{EO} = 0.01 millimol/lit, the following kinetic data were obtained in a batch reactor.

C_A, millimol /lit	0.84	0.53	0.27	0.09	0.018	0.0025
Time(t),h	1	3	5	7	9	11

Fit the above data using least square regression in Michaelis - Menten equation $-r_A = k_3 C_A C_{E0}/(C_A + M)$ and find Michaelis - Menten constant (M). [16]

8. Find the roots of the following function $f(x) = (2x-5)^4 - (x^2-1)^3$, using Newton-Raphson method. [16]

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Code No: 07A70804 **R07** **Set No. 1**

IV B.Tech I Semester Examinations,May 2011
PROCESS MODELING AND SIMULATION
Chemical Engineering

Time: 3 hours **Max Marks: 80**

Answer any FIVE Questions
All Questions carry equal marks

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1. Develop a mathematical model for isothermal CSTR in which an irreversible reaction $A \xrightarrow{k} B$ takes place. Assuming constant hold up in the reactor, discuss an algorithm for solving the modeled equations. [16]

2. (a) Fit a polynomial of second degree to the data points given in the following table:

x	0	1.0	2.0
Y	1.0	6.0	17.0

(b) Certain experimental values of x and y are given below:

x	0	2	5	7
y	-1	5	12	20

If $y = a_0 + a_1 x$, find approximate values of a_0 and a_1 using least square method. [8+8]

3. Write short note on:
   (a) Continuity equation.
   (b) Component continuity equation.
   (c) Energy equation.
   (d) Equation of motion. [4+4+4+4]

4. Suppose a mixture of gases is fed into a Gas-phase, pressurized CSTR, Gases are perfectly mixed. A reversible reaction occurs. The forward reaction is 1.5^{th} order in A; the reverse reaction is 1^{st} order in B. The mole fraction of A in the reactor is y. The pressure in the vessel is P. The volume of the reactor V is constant. Assume isothermal system, perfect gases. The feed stream has a density ℓ, mole fraction y_0 & flow rate F_0. The flow out of the reactor passes through a valve into another vessel which is held at a constant pressure P_D. Derive the mass balance and component continuity equations for the system. [16]

5. Consider the following non-linear algebraic equation to find the roots of $f(x) = x^3 - 5x^2 + 6x - 1$, using secant method. [16]

6. (a) Write all assumptions in deriving modeling equations of Binary distillation column.
   (b) Write the Model questions for "Top tray" and "next to top tray" in an ideal binary distillation column. [8+8]

7. A blend of 50% toluene liquid volume and 50%benzene liquid volume is being separated by fractionation into an overhead product that has 10.0 mole percent toluene and a bottom product that has 0.5 mole percent benzene. The blend is fractionated at the rate 10000 gal/day . How many gallons of each product is produced, if the reflux ratio is 4. A sample of vapour from one of the trays above the feed tray was taken and found to contain 20% toluene. What was the composition of the liquid from the tray along the point of which the sample of vapour was taken? [16]

8. Use the predictor - corrector formula for tabulating a solution of $10\frac{dy}{dx} = x^2 + y^2, y(0) = 1$ for the range $0.5 \leq x \leq 1.0$. Use R-K method to estimate the initial values. [16]

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Code No: 07A70804 **R07** **Set No. 3**

IV B.Tech I Semester Examinations,May 2011
PROCESS MODELING AND SIMULATION
Chemical Engineering

Time: 3 hours **Max Marks: 80**

Answer any FIVE Questions
All Questions carry equal marks

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1. (a) Define "Polynomial Interpolation".
   (b) Discuss about forward and backward differences. [6+10]
2. Explain the convergence procedure to find the bubble point temperature of a binary vapour-liquid mixture. [16]
3. (a) Explain ideal binary distillation with a neat sketch
   (b) Write the model equations for "nth tray" and "feed tray" in an ideal binary distillation column. [8+8]
4. Describe the simulation of Batch reactor using Runge-kutta Method. [16]
5. An irreversible exothermic reaction is carried out in a single perfectly mixed non-isothermal CSTR. The reaction is $A \rightarrow B$. The reaction is nth order in reactant A and has heat of reaction 'λ' (energy units/mole of A reacted). Negligible heat losses and constant densities are assumed. To remove the heat of reaction, a cooling jacket surrounds the reactor. Cooling water is added to the jacket at a constant volumetric flow rate. Develop a mathematical model for the system assuming that the CSTR has a significant metal wall capacitance. State all the assumptions made and explain the notations scheme used clearly. [16]
6. Consider the initial value problem $y^1 = x\,(y + x) - 2, y\,(0) = 2$, use Euler's Method with step sizes h=0.3, h=0.2 to compute approximations to y(0.6) [16]
7. Compare convergence time, using Newton-Raphson Method, for an ideal, four component vapour-liquid equilibrium system. The pure component vapour pressures are:

Component	Vapour Pressure (Psia) Pj	
	at 150^0 F	at 200^0 F
1	25	200
2	14.7	60
3	4	14.7
4	0.5	5

Calculate the correct temperature and vapour compositions for a liquid at 75 psia with a composition:
xl = 0.10
x2 = 0.54
x3 = 0.30

x4 = 0.06
Assume the system is ideal. [16]

8. (a) Define "Degrees of freedom" and explain the importance of it in process modeling.
   (b) Wrie applications of Raoult's law and Daltons law briefly. [8+8]

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