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

IV B.Tech I Semester Examinations,November 2010
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) 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]

2. (a) Write the component continuity equation for a CSTR in which a "simultaneous reaction" (first- order, isothermal) takes place $A \xrightarrow{K_1} B \xrightarrow{K_2} C$.
(b) Write component continuity equation for the same above system in which reversible reaction takes place instead of simultaneous reaction. [8+8]

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

4. Describe the simulation of Batch reactor using Runge-kutta Method. [16]

5. 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 and 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]

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

7. The height 'h' of a liquid in a gravity flow tank & the liquid velocity 'v' leaving through the outlet of the tank are given by the following equations $\frac{dv}{dt} = ph - qv^2$, $\frac{dh}{dt} = r - sv$, where p, q, r, s are constants. Explain the procedure to solve these equations for v and h by Runge-Kutta 4^{th} order method. [16]

8. Write the model equations involved in a Batch reactor when it is in the cooling phase with a neat diagram. [16]

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

IV B.Tech I Semester Examinations,November 2010
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) In a gas phase reversible reaction V_c moles of C react and form V_d moles of D. Derive an expression for chemical equilibrium and define the value of the equilibrium constant.
   (b) Briefly discuss about Raoult's law and its applications. [8+8]

2. Derive the equations describing the Batch distillation column with constant hold up. [16]

3. Consider a two perfectly mixed tanks in series, the flow rate of oil passing through the tanks is F, density ℓ, heat capacity C_p. The volume of 1^{st} tank is V_1 and 2^{nd} tank is V_2, which are constant. The temperature of oil entering 1^{st} tank is T_o. The temperatures in the two tanks are T_1 & T_2. A heating coil in the 1st tank uses steam to heat the oil. Write the energy balances for both the tanks. [16]

4. 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]

5. Given the following $f(x) = x^4 - x - 10$, $x_0 = 2$, Find the roots corrected to 3 decimal places using Newton-Raphson method. [16]

6. Using Euler's Method, solve the differential equations:
   (a) $\frac{dy}{dx} + 2y = 0, y(0) = 1$
   (b) $\frac{dy}{dx} - 1 = y^2, y(0) = 0$, Take h=0.1 and obtain y(0.1), y(0.2), y(0.3). [16]

7. Discuss the simulation of Non-isothermal CSTR using Euler's Method. [16]

8. Using Lagrange's Interpolation, obtain an appropriate third degree polynomial for the vapor pressure of acetone shown in table below, which could be used for 259.2K $\leq$ T $\leq$ 320.5K. [16]

T(K)	P^{sat} (bar)
259.2	0.04267
273.4	0.0949
290.1	0.2152
320.5	0.7444
350.9	2.015
390.3	5.65
446.4	17.68
470.6	26.62
508.1	47.00

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

IV B.Tech I Semester Examinations,November 2010
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. Explain the following methods:
   (a) Bisection Method.
   (b) False Position Method. [8+8]

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 n^{th} 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. Explain the convergence procedure to find the bubble point temperature of a binary vapour-liquid mixture. [16]

4. Simulate the series of three isothermal CSTRs using Runge-Kutta method. [16]

5. Explain the convergence procedure to find the bubble point temperature of a binary vapour-liquid mixture. [16]

6. Evaluate $I = \int_0^1 \frac{1}{1+x} dx$, correct to three decimal places. Solve this using trapezoidal rule with h=0.5, 0.25, 0.125 [16]

7. Derive the equation for the time required to achieve desired conversion in Batch reactor for Non-isothermal operation and Adiabatic operation. [16]

8. The reaction rate constant for the decomposition of a substituted dibasic acid has been determined at various temperatures as follows:

T (^{0}C)	50	70.1	89.4	101.0
K$\times 10^4$ (hr)	1.08	7.34	45.4	138

   Use the method of least squares to determine the activation energy (E) in the equation $k = Ae^{-E/RT}$, where T is measured in degree Kelvin. [16]

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

IV B.Tech I Semester Examinations,November 2010
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) Simulate the series of open loop three isothermal CSTRs using first order explicit Euler integration method.
   (b) Simulate the series of closed loop three isothermal CSTRs using first order explicit Euler integration method. [8+8]

2. 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]

3. (a) Define the terms "Modeling" and "Simulation".
   (b) Discuss the "Principles of formulation" in developing a mathematical model for a process. [6+10]

4. 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]

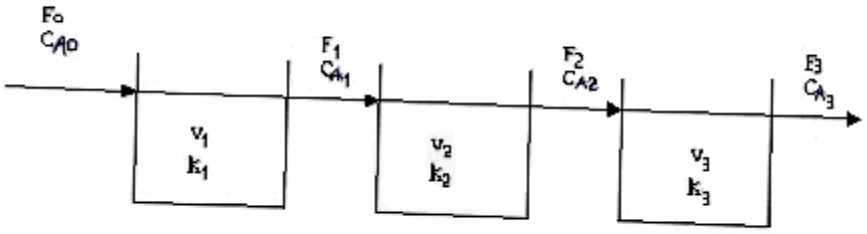

Figure 1:

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

6. Hot oil is cooled in a counter current heat exchanger, using cooling water as shown shown in figure 2:

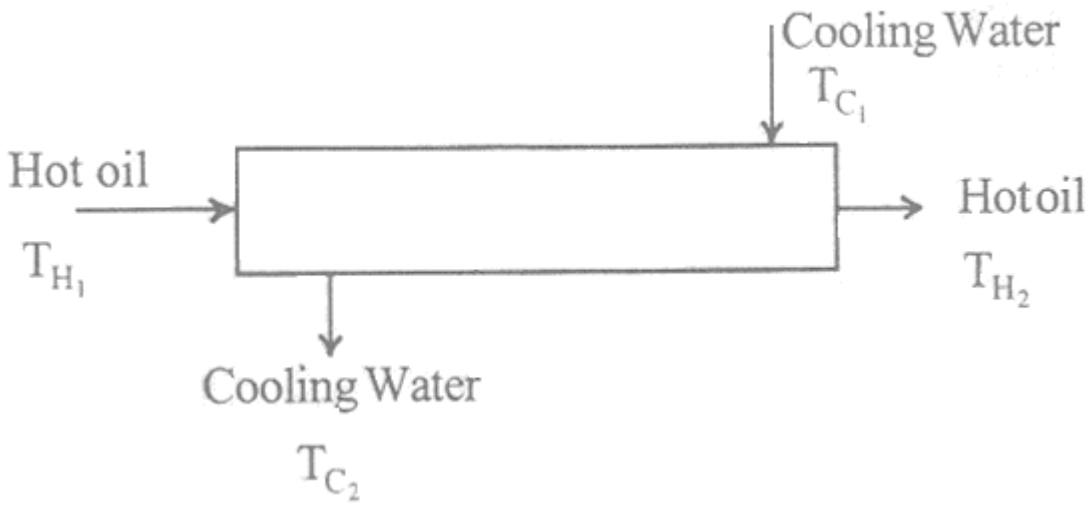

Figure 2:

The inlet temperatures of oil and cooling water, flow rates, heat transfer coefficients, and the heat transfer area are known. Describe the iteration steps for the calculation of steady state outlet temperatures of both the streams and the heat transfer rate. Give the relevant equations. [16]

7. Solve the following system by the Gauss Elimination Method:

$$2x + 2y + z + 2u = 7$$
$$x - 2y - u = 2$$
$$3x - y - 2z - u = 3$$
$$x - 2u = 0$$

[16]

8. The following table gives the effect of the aromatics concentration, C_A, on the rate, r_A, of coke formation on a metal plate during pyrolysis of naphtha in a jet stirred reactor, at 1083K.

10^4 C_A Kmol/m^3	1.79	2.03	2.22	2.47	2.97	3.39	4.95	7.37	9.01	9.83	10.07
10^2 r_A Kg/m^2 hr	0.28	0.32	0.36	0.4	0.49	0.59	0.99	1.55	2.0	2.25	2.6

Determine the order of the reaction using the expression $r_A = kC_A^n$ and least square fit ($\ln r_A = \ln k + n \ln C_A = a_0 + a_1 x$) [16]

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