Code No: RR410805 **Set No. 1**

IV B.Tech I Semester Regular Examinations, November 2005
PROCESS MODELLING & SIMULATION
(Chemical Engineering)

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

Answer any FIVE Questions
All Questions carry equal marks

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1. The liquid phase hydrolysis reaction of acetic anhydride to form acetic acid is carried out in a constant volume adiabatic batch reactor. The reaction is exothermic with the following stoichiometry. $(CH_3C)_2O + H_2O \rightarrow 2CH_3COOH + \text{Heat}$.
   Derive mass and energy balances for the system assuming the reaction as first order. [16]

2. Write the component continuity equations for the following reactions taking place in a CSTR (continuous stirred-tank reactor):

   (a) Simultaneous reactions (first-order, isothermal)
   $\mathbf{A} \overset{k_1}{\rightarrow} \mathbf{B}$ $A \overset{k_2}{\rightarrow} \mathbf{C}$

   (b) Reversible (first-order, isothermal)
   $\mathbf{A} \underset{k_2}{\overset{k_1}{\rightleftarrows}} \mathbf{B}$

   State the assumptions made and explain the nomenclature used. [16]

3. An irreversible exothermic reaction is carried out in a single perfectly mixed non-isothermal CSTR. The reaction is A → B. The reaction is nth order in reactant A and has heat of reactλ (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 perfectly mixed cooling jacket. State all the assumptions made and explain the notation scheme used clearly. [16]

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

5. Derive the Mathematical Model equations for a Binary distillation column. [16]

6. Under numerical integration methods of ordinary differential equations, discuss about the explicit Euler algorithm in detail. Compare it with implicit Euler algorithm. Write about their relative advantages and disadvantages. [16]

7. Develop a mathematical model for a simple gravity flow tank into which an incompressible liquid is pumped at a variable flow rate of F_o (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 is h (m) .The flow rate out of the tank is F (m^3/s).Discuss the Newton-Raphson algorithms for solving the modeled equations. [16]

8. Discuss the general "Newton - Rapshan" algorithm to determine the bubble point temperature for a binary system of components 1 and 2. Assume the system is ideal, Raoult's and Dalton's laws are applicable. [16]

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1. Write short notes on:
   (a) Law of conservation of momentum
   (b) Transport laws
   (c) Equations of state [16]

2. Referring to the figure shown below, write the force balance equation for the liquid flowing through the pipe of cross sectional area A_p (m^2) and length L (m). The velocity of the liquid flow through the pipe is v (m/s). The vertical cylindrical tank has a cross-sectional area of A_T (m^2). The density of the liquid is ρ (kg/m^3). Assume the flow is turbulent, plug flow and the fluid is incompressible. State any other assumptions you make and explain the notation scheme used clearly.as shown in the figure1 below

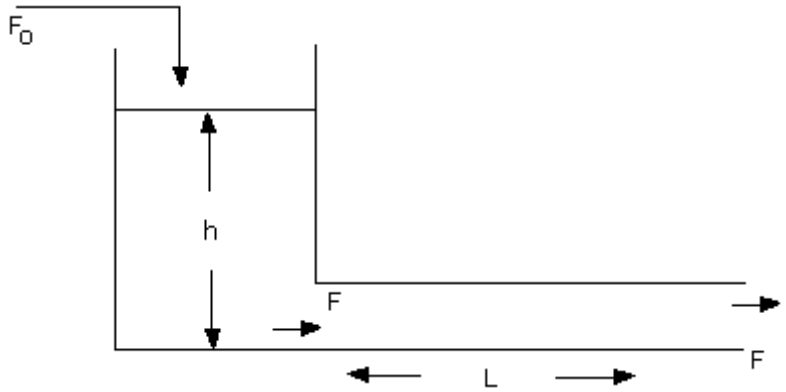

Figure 1:

[16]

3. Consider the CSTR process shown in the (figure2) given below. Both a liquid product stream F and a vapour product stream F_v (volumetric flow) are withdrawn from the vessel. The pressure in the reactor is P. Vapour and liquid volumes are V_v and V. The density and temperature of the vapour phase are ρ_v and T_v. The mole fraction of A in the vapour is y. If the phases are in thermal equilibrium, the vapour and liquid temperatures are equal ($T = T_v$). If the phases are in phase equilibrium, the liquid and vapour compositions are related by Raoult's law, a relative volatility relationship or some other vapor-liquid equilibrium relationship. The enthalpy of the vapour phase H (cal/g) is a function of composition y, temperature T_v, and

pressure P. Neglecting kinetic energy and potential energy terms and the work term write the energy equation for the system. State the assumptions made and explain the notation scheme used.

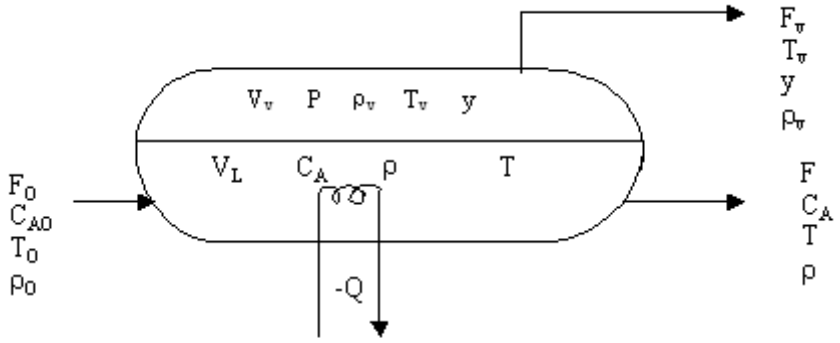

Figure 2:

[16]

4. Explain the steady state model and thermal equilibrium model for LPG vaporiser with a neat diagram. [16]

5. Derive the Mathematical Model equations for a Binary distillation column. [16]

6. Under numerical integration methods of ordinary differential equations, discuss about the explicit Euler algorithm in detail. Compare it with implicit Euler algorithm. Write about their relative advantages and disadvantages. [16]

7. Develop a mathematical model for a Non-isothermal CSTR in which an exothermic reaction $A \rightarrow B$ takes place. The reactor is provided with a cooling jacket for the removal of heat. Assume constant holdup in the reaction vessel. Discuss an algorthim for solving the model equations. [16]

8. Discuss the general "Newton - Rapshan" algorithm to determine the bubble point temperature for a binary system of components 1 and 2. Assume the system is ideal, Raoult's and Dalton's laws are applicable. [16]

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1. Write
   (a) Total continuity equation (mass balance)
   (b) Component continuity equation (component balance) and
   (c) Energy equation. Explain the notation scheme used and state the assumptions made clearly. [16]

2. Referring to the figure shown below, write the force balance equation for the liquid flowing through the pipe of cross sectional area A_p (m^2) and length L (m). The velocity of the liquid flow through the pipe is v (m/s). The vertical cylindrical tank has a cross-sectional area of A_T (m^2). The density of the liquid is ρ (kg/m^3). Assume the flow is turbulent, plug flow and the fluid is incompressible. State any other assumptions you make and explain the notation scheme used clearly.as shown in the figure1 below

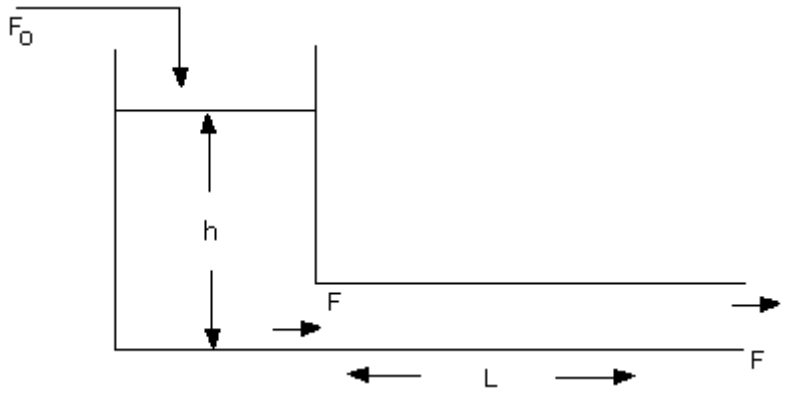

Figure 1:

[16]

3. A first order irreversible exothermic reaction A → B occurs in a series of three perfectly mixed CSTRs. Feed enters the first reactor and product leaves the third reactor. Derive the mass balance and component continuity equations considering isothermal and constant holdups. Assume constant density for the system, which is a binary mixture of A and B. [16]

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

5. Derive the Model equations to describe the Batch distillation of a multicomponent mixture. [16]

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

7. Develop a mathematical model for the perfectly mixed reactor in which a first order irreversible reaction with specific rate constant k is taking place as per the reaction

$$A \xrightarrow{k} B$$

Discuss the algorithm to solve the equations by Runge kutta method. [16]

8. Develop a mathematical model for a counter current double pipe heat exchanger process for predicting the transient response. Discuss an Euler algorithm for solving the model equations. Give a suitable flow chart for the simulation. [16]

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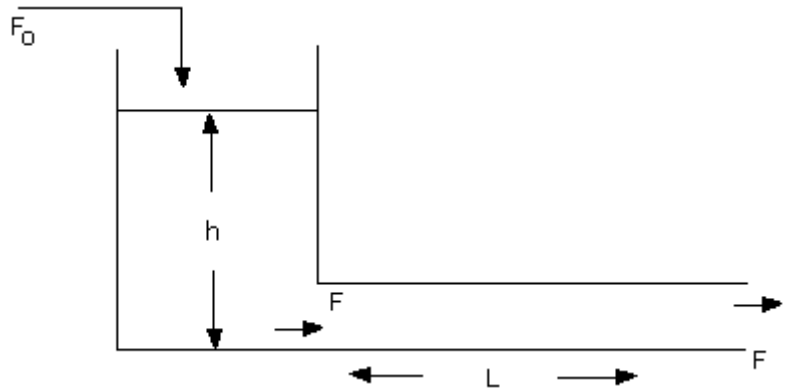

Figure 1:

[16]

3. An irreversible exothermic reaction A→ B occurs in a series of three perfectly mixed CSTRs. Feed enters the first reactor and product leaves the third reactor. Assume the reaction is nth 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]

4. Explain the steady state model and thermal equilibrium model for LPG vaporiser with a neat diagram. [16]

5. Derive the Mathematical Model equations for a Binary distillation column. [16]

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

7. Develop a mathematical model for a system of three ideal CSTRs (isothermal) connected in series. Draw an anolog computer simulation circuit diagram for solving the model equations. [16]

8. Develop a mathematical model for a binary distillation column for predicting the transient response. Discuss an algorithm for solving the model equation. Give a suitable flow chart for the simulation. [16]

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