Code No: M0824/R07 **Set No. 1**

IV B.Tech. I Semester Supplementary Examinations, February/March - 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. Write the total and component continuity equations for the following reactions taking place in a CSTR (continuous stirred-tank reactor):
   a) Simultaneous reactions (first-order, isothermal) $A \xrightarrow{k_1} D \xrightarrow{k_2} C$
   b) Reversible (first-order, isothermal) $A \xrightarrow{k_1} B$, $B \xrightarrow{k_2} A$
   State the assumptions made and explain the nomenclature used.

2. a) Explain in detail the use of mathematical models.
   b) Derive the energy equation applicable for a stirred tank reactor. State the assumptions clearly.

3. Derive a Mathematical Model for the Batch reactor in which the First order consecutive reactions $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ takes place to get the product B.

4. a) Solve the following equations by Gauss-Elimination method
   10x+y+z=12, 2x+10y+z=13, x+y+5z=7
   b) Solve $x^3 + 2x^2 + 10x - 20$ by Newton-Raphson method (initial guess xo=1.2)

5. a) Solve $\frac{dy}{dx}$ = (x+y)y, y(0) =1 using Milne's Predictor-corrector method for y(0.4). The values y(0.1)=1.11689; y(0.2)=1.27739; y(0.3) = 1.50412
   b) $\frac{dy}{dx} = x^2 + y^2$ with y(0) = 0. Estimate y (0.4) by using R-K fourth order method. Take h=0.2

6. The following table gives the distance in nautical miles of the visible horizon for the given heights in feet above the earth's surface:

X=height	100	150	200	250	300	350	400
Y=distance	10.63	13.03	15.04	16.81	18.42	19.9	21.27

Find the values of y when (i) x=218 ft (ii) x=410 ft.

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Set No. 1

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

8. Discuss the general "Newton - Raphson" 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.

Code No: M0824/R07 **Set No. 2**

IV B.Tech. I Semester Supplementary Examinations, February/March - 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. Write the component continuity equations for a perfectly mixed batch reactor (no inflow or outflow) with first-order isothermal reactions:
   i) Consecutive
   ii) Simultaneous
   iii) Reversible

2. 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 react 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 plug flow cooling jacket. State all the assumptions made and explain the notations scheme used clearly.

3. Derive the Mathematical Model equations for a Binary distillation column

4. a) Find one root of the $x^3-3x+1=0$ using Newton-Raphson method
   b) Determine the Eigen values and Eigen vectors of

$$A = \begin{bmatrix} 6 & -2 & 2 \\ -2 & 3 & -1 \\ 2 & -1 & 3 \end{bmatrix}$$

5. a) $\frac{dy}{dx} = 3x + 1$ with y(1) = 2. Estimate y(2) by Euler's method using
   i) h=0.5
   ii) h=0.25
   b) Evaluate $\int_0^1 \frac{dx}{1+x^2}$ by using Trapezoidal rule taking h=0.1

Set No. 2

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6. a) Fit a third degree polynomial through these points using the Lagrangian Interpolation formula find y(5)

X	1	3	4	6
Y	7	53	157	857

b) Fit a second degree parabola to the following data.

x	1	1.5	2	2.5	3	3.5	4
y	1.1	1.3	1.6	2	2.7	3.4	4.1

7. Develop a mathematical model and discuss the general algorithm by Euler method for a perfectly mixed tank in which the reactant A gives B at a specific rate constant k1, at the same time B gives C with a rate constant k2 as per the reaction.

$A \xrightarrow{k_1} B \xrightarrow{k_2} C$

8. Discuss the general "Newton - Raphson" 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.

Code No: M0824/R07 **Set No. 3**

IV B.Tech. I Semester Supplementary Examinations, February/March - 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. Consider a continuous stirred tank reactor in which a chemical reaction is taking place in the liquid in the tank. Component A reacts irreversibly and at a specific reaction rate k to form product, component B.

$$A \xrightarrow{k} B$$

The concentration of component A in the inflowing feed stream be C_{AO} and in the reactor C_A. Assuming a simple first order reaction, the rate of consumption of reactant A per unit volume will be directly proportional to the instantaneous concentration of A in the tank. Write the component continuity equations (component balances) and the total continuity equation (mass balance) for the above system.

2. 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

3. Explain the steady state model and Liquid phase dynamics model for LPG vaporizer with a neat diagram

4. a) Find a real root of the equation $x^3 - 2x - 5 = 0$ by the method of false position
   b) Determine the Eigen values and Eigen vectors of

$$A = \begin{bmatrix} 6 & -2 & 2 \\ -2 & 3 & -1 \\ 2 & -1 & 3 \end{bmatrix}$$

5. a) Using Euler's method, compute y(1) from $\frac{dy}{dx} = 10(x^2 + y^2)$, y(0)=1,h=0.1
   b) Evalute $\int_0^6 \frac{dx}{1+x^2}$ by using Simson's 1/3 rule taking h=1

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Set No. 3

6. a) The following table gives the values of density of saturated water for various temperature of saturated steam.

Temp(^oC)	100	150	200	250	300
Density(kg/m^3)	958	917	865	799	712

Find by interpolation, the densities when the temperatures are 130^{o}C and 275 ^{o}C respectively.

b) Fit a straight line to the following data.

X	1	2	3	4	5
Y	14	27	40	55	68

7. Develop a mathematical model for a gravity flow tank into which an incompressible liquid is pumped at a variable flow rate of Fo (m3/s) .This inflow rate can vary with time because of changes in operations in the upstream The height of the liquid in the vertical cylindrical is h (m). The flow rate out of the tank is F (m3/s).Discuss the Explicit first order Euler method for solving the modeled equations

8. Discuss an algorithm for solving the model equations of Non-isothermal CSTR in which an exothermic reaction A→ B takes place. The reactor is provided with a cooling jacket for the removal of heat. Assume constant holdup in the reaction vessel.

Code No: M0824/R07 **Set No. 4**

IV B.Tech. I Semester Supplementary Examinations, February/March - 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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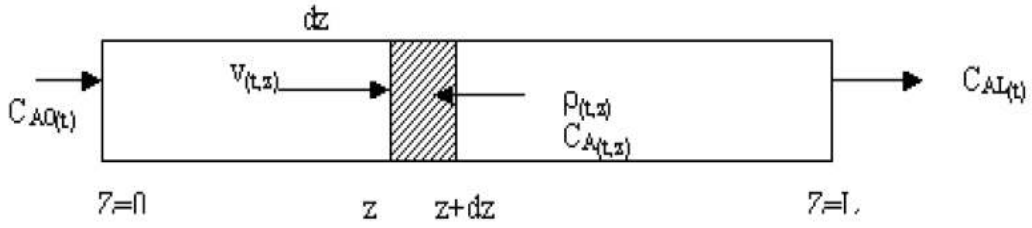
1. Consider a tubular reactor in which the following reaction takes place. Component A reacts irreversibly and at a specific reaction rate k to form product, component B.

$$A \xrightarrow{k} D$$

As a slice of material moves down the length of the reactor the concentration of the reactant CA decreases as A is consumed. Density, ρ velocity v, and concentration C_A can all vary with time and axial position z. Assume plug flow conditions so that there are no radial gradients in velocity, density or concentration. Apply the component continuity equation for the reactant A. State all the assumptions made and explain clearly the nomenclature used. as shown in the figure below



2. 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

3. Explain the steady state model and Liquid phase dynamics model for LPG vaporizer with a neat diagram

4. a) Find a real root of the equation $x^3 - 2x - 5 = 0$ using bi-section method
   b) Solve x+y+z = 1; 3x+y-3z = 5; x-2y-5z = 10 by Gauss Jordon method.

5. a) Using Euler's method,Compute y(1) from $\frac{dy}{dx} = 10(x^2 + y^2)$, y(0)=1,h=0.1
   b) Evalute $\int_0^6 \frac{dx}{1+x^2}$ by using Simson's 1/3 rule taking h=1

Set No. 4

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6. a) Use Lagrange's interpolation formula to find the value of y when x =10, if the values of x and y are given as below:

x	5	6	9	11
y	12	13	14	16

(b)Fit a power-function model of the form $y = a.x^b$, for the given data

x	1	2	3	4	5
y	0.5	2	4.5	8	12.5

7. The height h of a liquid in a gravity flow tank and 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** and **s** are constants. Explain the procedure to solve these equations for v and h by fourth order Runge – Kutta method

8. Discuss an algorithm for solving the model equations of Non-isothermal CSTR in which an exothermic reaction A→ B takes place. The reactor is provided with a cooling jacket for the removal of heat. Assume constant holdup in the reaction vessel.