B.TECH / CHE /7[TH] SEM/ CHEN 4103/2017

MODELING, SIMULATION AND OPTIMIZATION
(CHEN 4103)

Time Allotted : 3 hrs **Full Marks : 70**

Figures out of the right margin indicate full marks.

Candidates are required to answer Group A and any 5 (five) from Group B to E, taking at least one from each group.

Candidates are required to give answer in their own words as far as practicable.

Group – A
(Multiple Choice Type Questions)

1. Choose the correct alternative for the following: **10 × 1 = 10**

(i) Trace quantities of impurities in feed can be best removed by
(a) purging
(b) reacting in separate reactions
(c) separating in a separation vessel
(d) none of these.

(ii) When there is appreciable boiling point elevation, optimal number of evaporator effects is
(a) 8-10 (b) >10 (c) ≤ 6 (d) cannot be determined.

(iii) A and B are reacting where B is a toxic chemical. An ideal distribution of chemicals would involve
(a) using excess B
(b) using excess A
(c) using an inert species C
(d) using stoichiometric amounts of A and B.

(iv) Pressure drop for a low-viscosity liquid in a heat exchanger can be estimated to be
(a) 1.5 psi (b) 5 psi (c) 3 psi (d) 7-9 psi.

(v) Which kind of reactor is widely used for noncatalytic homogeneous reactions?
(a) CSTR (b) Laminar flow reactor
(c) Fluidized bed reactor (d) Tubular reactor.

(vi) Crystal growth rate is controlled by
(a) limiting the extent of supersaturation
(b) crystallization temperature
(c) crystallization technique
(d) nature of the crystal.

(vii) Selectivity in zeolite adsorbents is controlled by
(a) adsorption equilibrium (b) adsorption temperature
(c) adsorption pressure (d) molecular sieving.

(viii) Which kind of reactor is most suitable for an isothermal homogeneous liquid phase reaction?
(a) CSTR (b) PFR
(c) Tubular reactor with axial dispersion (d) Laminar flow reactor.

(ix) Slack variables
(a) are needed in Newton's method of finding the optima
(b) are a part of the conjugate gradient method
(c) are additional constraints in linear programming
(d) none of the above.

(x) Golden search algorithm divides the space between the upper and lower bound
(a) in the ratio $(\sqrt{5}-1)/3$ (b) in the ratio $(\sqrt{5}-1)/3$
(c) in the ratio 2:3 (d) none of these.

Group - B

2. (a) What are the advantages of modular approach over equation oriented approach with respect to flowsheeting? What are the characteristics of a flowsheet module?

(b) Suppose the following table is obtained after calculation of output flow rates in a distillation column separating benzene, toluene and Xylene:

Component	Input flow	Top output flow	Bottom output flow
Benzene	100 mol	97 mol	1 mol
Toluene	100 mol	95 mol, 2 mol Benzene	5 mol
Xylene	100 mol	7 mol	93 mol
Heat	20,000 kJ	13,000 kJ	7,000 kJ

Write an expression for benzene top outflow as a linear function of input flows of all the components.

(3 + 3) + 6 = 12

3. (a) Two exothermic liquid-liquid reactions are taking place, one with $\Delta H = -23000$ kJ/mol, another with $\Delta H = -15360$ kJ/mol. Will you use the same measure for temperature control in both cases? If not, then what measures can you adopt for temperature control for both reactions?

(b) A gas (with $\gamma = 1.4$) is to be compressed from 20 psia to 500 psia. How many compression stages will be required? What will be the values of the inlet and outlet pressures for each stage if we want to ensure optimal inter-stage pressures? (Assume a 2-psi pressure drop for each inter-stage cooler.)

4 + (3 + 5) = 12

Group - C

4. (a) What are the assumptions of the ideal PFR reaction model?

(b) Explain how the PFR model can be applied to i) noncatalytic homogeneous reactions and ii) fixed bed catalytic reactors. Why the CSTR model cannot be applied for a fluidized bed catalytic reactor?

4 + (6 + 2) = 12

5. (a) What is the significance of attainable region in reactor network synthesis? What is meant by a convex attainable region?

(b) For the reaction scheme given below, write the equations that need to be solved for constructing a PFR trajectory. How can a PFR trajectory be expanded?

$$A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B \xrightarrow{k_3} C$$
$$2A \xrightarrow{k_4} D$$

(3+3) + (3+4) = 12

6. (a) Suppose y[illegible] ave the option to install structured packings, random packings and valve trays. Which option will be most preferable to you? Justify your answer.

(b) A chemical reaction is taking place simultaneously with distillation. In your distillation column, which type of tray will you want to install: sieve tray, valve tray or bubble cap tray? Justify your answer.

(c) What are the different guidelines by which you can select the type of condenser and cooling medium for a distillation column?

3 + 3 + 6 = 12

7. (a) What type of distillation column (tray/packed) will you select for an operation which involves: (i) corrosive systems (ii) Large column diameter (iii) High liquid/gas ratio.

B.TECH / CHE / 7TH SEM / CHEN 4113 / 2017

(b) In case of a liquid-liquid extraction operation which type of equipment will you select for (i) operation which requires only a few theoretical stages (ii) operation requiring a large number of stages?

(c) Mention four important factors which influence the selection of the type of dryer.

6 + 2 + 4 = 12

Group - E

8. (a) A batch distillation unit has two types of column: Type 1 and Type 2. If required, all Type 1 columns and all Type 2 columns can be operated simultaneously, and total available operating time is 6000 hrs per week for Type 1 columns and 10000 hrs per week for Type 2 columns. It is desired to use these columns to manufacture two different products A and B. Distillation time to produce 100 gal of product A is 2hr in Type 1 columns and 1 hr in Type 2 columns. Distillation time to produce 100 gal of product B is 1 hr in Type 1 columns and 4 hr in Type 2 columns. The net profit is Rs 50/gal for product A and Rs 30/gal for product B. It is required to find the production schedule that maximizes the net profit in Rs/week.

Formulate the objective function with all constraints and bounds.

(b) Use any suitable optimization method to solve the problem. Illustrate the feasible region with a graph.

7 + 5 = 12

9. (a) For the purposes of planning you are asked to determine the optimal heat exchanger areas for the sequence of three exchangers as shown in fig.1.

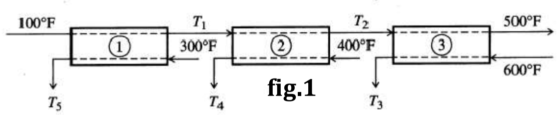

fig.1

You are also given:

Heat Exchanger	U (overall ht tr coeff) cal/(hr m² deg K)	Area
1	120	A_1
2	80	A_2
3	40	A_3

Given $mC_p = 10^5$ cal/h°K

What are the design variables? Formulate the objective function and all constraints and bounds.

(b) Are there any non-linearities in the above problem? If so, where? Write out the first order and second order conditions necessary for optimality.

6 + (3 + 3) = 12