

**MODELING SIMULATION & 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) Which of the following is a process for separating vapour mixtures?
(a) Crystallization
(b) Azeotropic distillation
(c) Adsorption
(d) Stripping.
- (iii) Packed columns are superior to tray columns in case of
(a) large diameter column
(b) high L/G ratio
(c) initial installations
(d) vacuum operations.
- (iv) For developing heads up to 3200 ft we should use a
(a) Diaphragm pump
(b) Centrifugal pump
(c) Plunger pump
(d) Peristaltic pump.
- (v) Selectivity in activated carbon adsorbents is controlled by
(a) Adsorption equilibrium
(b) Nature of adsorbate
(c) Porosity of adsorbent
(d) Molecular sieving.
- (vi) Linear Programming Problem was discovered by
(a) Simplex (b) Shuler (c) Dantzig (d) Aris.
- (vii) The first moment for Residence Time Distribution in a chemical real reactor is
(a) a function approaching zero
(b) mean residence time
(c) a function approaching infinity
(d) variance.

- (viii) For drying small free flowing particles we should use
(a) Rotary dryer
(b) Fluidized bed dryer
(c) Pneumatic conveying dryer
(d) Spray dryer.
- (ix) Cryogenic distillation is feasible for gas separation when relative volatility between key components is
(a) < 1 (b) >1 but <2 (c) = 2 (d) >2.
- (x) The concept of Attainable Region Theory helps one to address
(a) The reactor network synthesis problem
(b) Reactor Economy
(c) Reactor Material of Construction
(d) None of the above.

Group – B

2. (a) What are the advantages of modular approach over equation oriented approach with respect to flowsheeting? What is the difference between a process module and a processing unit?
- (b) The following reaction takes place in a chemical processing unit:

$$A + B + S \rightarrow C + D + S$$
 The heat of reaction is $\Delta H = -34365$ kJ/mol. Cost of separation of inert species S from feed is Rs 300/kmol of S separated while the cost of separation from product stream is Rs 400/kmol of S. The company has enough capital to provide for a large reactor. Develop the flowsheet of the process keeping in mind the following considerations:
 (i) Valuable species E (in liquid state) is produced via a side reaction in trace quantities
 (ii) D is the desired product
 (iii) D is a vapor while C is a liquid
- (3 + 2) + 7 = 12**
3. (a) A pump is to be installed in a pipeline to pump 100 gpm of liquid water to a distance of 500 ft. There are 2 control valves in the pipeline and at one point, the pipeline is elevated by 6 ft. The pump draws water from the surface of a tank, open to atmosphere and the discharge pressure is fixed to be 1500 psi. What horsepower pump will be required?
- (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. Also if the gas flowrate is 20 ft³/min at 45°F and 1.5

atm, calculate the theoretical horsepower required for compressing the gas from 20 psia to 500 psia.

$$4 + 8 = 12$$

Group - C

4. (a) Show that for a Laminar Flow Real Reactor:

$$E(t) = 0 \text{ for } t < \frac{\tau}{2} \text{ and } \frac{\tau^2}{2t^3} \text{ for } t \geq \frac{\tau}{2}$$

- (b) Applying Danckwert's boundary conditions in Dispersion Model of a First order reaction for a suitable system, show that the molecules traveling on the streamline at $r = 3R/4$ exited the reactor at time $\frac{8}{7}\tau$.

$$6 + 6 = 12$$

5. (a) Discuss the concept of Attainable Region using geometric and mathematical optimization techniques to assist in the design chemical reactors network.

- (b) A Differential Side-stream Reactor (DSR) is represented by the following differential equation:

$$dC/dr = r(C) + \alpha(C)(C_0 - C), \text{ where } 0 \leq \alpha \leq \infty.$$

(symbols stand for usual notations).

Explain the methodology of construction of DSR with Schema, trajectory and the space spanned by a rate vector and mixing vector.

$$6 + 6 = 12$$

Group - D

6. (a) What do you understand by the term "separation factor" in connection with separation processes? Deduce an expression for separation factor for a binary distillation column.

- (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 large number of stages.

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

$$(3 + 2) + 4 + 3 = 12$$

7. (a) A feed containing components A, B, C and D is fed to a series of ordinary distillation columns. The product specifications are 98%

purity for each component. The flowrate of each component is given below:

A - 50 kmol/hr

B - 150 kmol/hr

C - 200 kmol/hr

D - 350 kmol/hr

Relative volatilities between each pair of components is also given:

A-B 3.5

B-C 1.8

C-D 2.5

Determine the most favourable sequence of separations in the columns and justify your answer.

- (b) Write a note on the applicability of partial condensation and cryogenic distillation as separation methods for gas mixtures.

$$8 + 4 = 12$$

Group - E

8. (a) Solve the following formulations:

$$x_1 - x_2 \geq -1; -0.5x_1 + x_2 \leq 2; x_1, x_2 \geq 0, \max z = 2x_1 + 2x_2$$

Prove that: Hyperplane is a Convex set.

- (b) For a system of Linear Inequalities with objective function Minimize $P(x) = -4x_1 - 5x_2$.

$$\text{Subject to constraints } x_1 - 2x_2 \leq 2; 2x_1 + x_2 \leq 6; x_1 + 2x_2 \leq 5; -x_1 + x_2 \geq 2$$

Discuss the algorithm to develop Simplex Method through different canonical forms.

$$(3 + 2) + 7 = 12$$

9. Minimize $x_0 = x_1^2 + x_2^2 + x_3^2$, subject to $4x_1 + x_2^2 + 2x_3 - 14 = 0$.

$$12$$