# SPECIAL SUPPLE B.TECH/CHE/7<sup>TH</sup> SEM/CHEN 4103/2018

## 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 <u>any 5 (five)</u> from Group B to E, taking <u>at least one</u> 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 ( (a) purging (c) separating in	of impurities in feed ca a separation vessel	in be best removed (b) reacting in sep (d) none of these	l by arate reactions
	(ii)	When there is an evaporator effect (a) 8-10 (c) ≤ 6	opreciable boiling points is	nt elevation, optin (b) >10 (d) cannot be det	nal number of termined.
	(iii)	For heat exchang approach is (a) 10°F	ge at temperatures up (b) 20°F	oto 300°F, optima (c) 50°F	l temperature (d) 80°F.
	(iv)	Pressure drop f approximately (a) 1.5 psi	for a low-viscosity l (b) 5 psi	iquid in a heat (c) 3 psi	exchanger is (d) 7-9 psi.
	(v)	For noncatalytic widely used? (a) CSTR (c) Fluidized bed	homogeneous reacti reactor	ions, which kind (b) Lamina (d) Tubular	of reactor is r flow reactor r reactor.
	(vi)	Packed columns a (a) Large diamete (b) Initial installa	are superior to tray col er column tions	lumns in case of (b) high L/( (d) vacuum	G ratio operations.

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#### (vii) Optimization studies are necessary when

- (a)  $N_{variables} > N_{equations}$
- (c)  $N_{\text{variables}} > N_{\text{decision variables}}$

(b)  $N_{variables} < N_{equations}$ 

(d)  $N_{variables} = N_{equations}$ 

## (viii) Newton's method of finding the maxima

- (a) is used in multivariable optimization
- (b) is based on the gradient of the objective function
- (c) both (a) and (b)
- (d) is an iterative process.
- (ix) Nonlinear programming is needed when
  - (a) the objective function is nonlinear in design variables
  - (b) constraints are nonlinear in design variables
  - (c) both (a) and (b)
  - (d) none of the above.
- (x) A saddle point
  - (a) is also called a minmax point
  - (b) makes gradient based search easy
  - (c) both (a) and (b)
  - (d) contains the local minima.

#### Group – B

- 2. (a) What are the drawbacks of the modular approach of flowsheeting compared to the equation oriented approach?
  - (b) Explain the significance of degrees of freedom in a flowsheet. Calculate the degrees of freedom for a mixing module where two inlet streams are mixed to give a single outlet stream. State any necessary assumptions.

4 + (2 + 6) = 12

- 3. (a) Two exothermic reactions are taking place, one with  $\Delta H = -2300 \text{kJ/mol}$ , another with  $\Delta H = -45360 \text{ kJ/mol}$ . 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.

$$4 + 8 = 12$$

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

$$A \stackrel{k_{1,k_{2}}}{\longleftrightarrow} B \stackrel{k_{3}}{\to} C$$
$$2A \stackrel{k_{4}}{\to} D$$

(b) For the reaction  $CO + 2H_2 \rightarrow CH_3OH$ , if an initial feed of 100 kmol/hr CO and 600 kmol/hr H<sub>2</sub> is given and there is 70% conversion of CO, what will be the molar flow rates of the components in the reactor effluent?

(3+3)+6=12

# Group – D

- 6. (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) 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?

6 + 4 + 2 = 12

- 7. (a) What are the conditions which ensure that only ordinary distillation columns will suffice for separation of hydrocarbon mixtures?
  - (b) Write a note on membrane separation by gas permeation.

6 + 6 = 12

## Group – E

- 8. (a) A batch distillation unit has two types of column: Type 1 and Type 2. Type 1 columns are available for 6000 hr/year while Type 2 columns are available 10000 hr/year. It is desired to use these columns to manufacture two different slates of 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/year. 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 Figure.



You are also given

Heat Exchanger	U (overall ht tr coeff) cal/(hr m <sup>2</sup> deg.K)	Area
1	120	A1
2	80	A <sub>2</sub>
3	40	A <sub>3</sub>

Given  $mC_p = 10^5 \text{ cal/h}^\circ\text{K}$ 

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

(b) Find out the optimal heat exchanger area for the sequence of heat exchangers.

6 + 6 = 12