

**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) For a reactive distillation operation which type of tray is most suitable?  
(a) Bubble cap (b) sieve  
(c) Valve (d) Linde.
- (ii) vant Hoff equation is given by \_\_\_\_\_, where 'k' is the equilibrium constant, 'T' is the temperature,  $\Delta H_{Rxn}^0$  is the heat of reaction at standard temperature and pressure.  
(a)  $\left(\frac{d\ln K}{dT}\right)_P = \frac{\Delta H_{Rxn}^0}{RT^2}$  (b)  $\left(\frac{d\ln K}{d\ln T}\right)_P = \frac{\Delta H_{Rxn}^0}{RT^2}$   
(c)  $\left(\frac{d\ln K}{dT}\right)_P = \frac{\Delta H_{Rxn}^0}{RT}$  (d)  $\left(\frac{dK}{dT}\right)_P = \frac{\Delta H_{Rxn}^0}{RT^2}$
- (iii) In case with the "inert diluent" arrangement for the temperature control of a reactor, after separation \_\_\_\_\_ is recycled back to the reactor through a heat exchanger.  
(a) part of the reactant (b) product  
(c) solvent (d) (a) and (c)
- (iv) Golden section search technique with the minimization problem is \_\_\_\_\_  
(a) an open ended algorithm (b) a method with lower and upper bound  
(c) providing local minima (d) (a) and (c)
- (v) Slack variables introduced in LP are also called \_\_\_\_\_ variables  
(a) non-basic (b) leaving  
(c) basic (d) either (b) or (c)
- (vi) During flow-sheeting by sequential modular approach, \_\_\_\_\_ would not need specification of equipment parameters.  
(a) Mixing tank (b) CSTR  
(c) Absorption column (d) Dryer

- (vii) A and B are reacting where B is a hazardous 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
- (viii) For developing heads upto 20,000 ft we should use a \_\_\_\_\_ .  
(a) Plunger pump  
(b) Centrifugal pump  
(c) Gear pump  
(d) Peristaltic pump
- (ix) \_\_\_\_\_ is an incident in Branch and Bound method for MIP, where the decision variables become integers with a definite value for an subproblem objective function.  
(a) Branching  
(b) Bounding  
(c) Fathoming  
(d) Degeneracy
- (x) Distillation column pressure is generally set according to the \_\_\_\_\_ .  
(a) cooling water temperature in condenser  
(b) nature of the components  
(c) reboiler heat duty  
(d) boiling point of light key

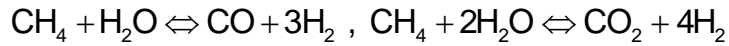
**Group – B**

2. (a) What are the characteristics of a flowsheet module? Which flowsheeting algorithm is generally followed in simulation softwares like ASPEN, DWSIM etc.?  
(b) Take a simple case of i) first mixing of benzene and toluene ii) subsequent separation of benzene and toluene by distillation. Draw the flow-sheet and develop the linear relationships among output and input variables as per simultaneous modular approach. Assume anything that you need logically.  
**4 + 8 = 12**
3. (a) In a countercurrent heat exchanger, a hot liquid A is being cooled by a cold liquid B. The inlet temperatures of A and B are 80°C and 30°C respectively. The mass flow rate of A and B is 5000 kg/hr. The specific heat capacities of A and B are 2 J/Kg.K and 1.8 J/Kg.K respectively. What will be the exit temperatures of A and B?  
(b) A vapour feed is being fed to a catalytic tubular reactor from where a vapour product is coming out. The feed contains some inerts which negatively impact the catalyst performance. The reaction is highly exothermic. The cost of separation of the inerts from feed is Rs. 2000/g while the cost of separation from the product is Rs. 500/g. Draw the flow-sheet of the process and justify it.  
**6 + 6 = 12**

**Group – C**

4. (a) In a steam reforming of methane unit, for the following reactions show that the total molar change of the components in the reactions can be expressed by the

twice of the molar change in CO<sub>2</sub>. Assume CO and CH<sub>4</sub> are the independent components.



- (b) For a reaction, comment on the stability of the system based on the feed temperature, when a and a' are two cases of heat removal condition for the utility as shown in the below figure 1.

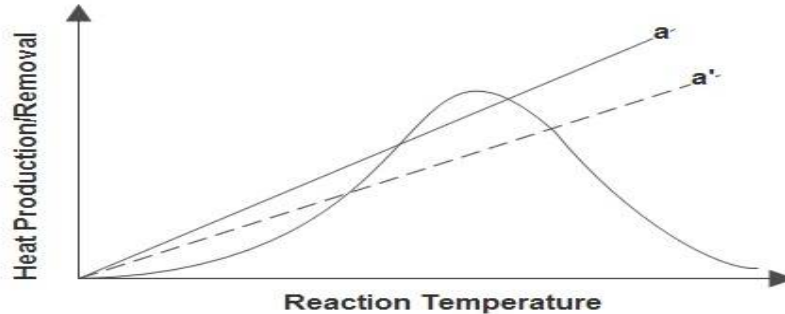
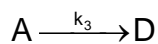
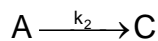
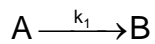


Fig. 1

8 + 4 = 12

5. (a) A system of three parallel reactions is:



$k_1 = 0.025 \text{ mol/L-min}$ ,  $k_2 = 0.2 \text{ min}^{-1}$ , and  $k_3 = 0.4 \text{ L/mol-min}$ , and the initial concentration of  $C_A = 1 \text{ mol/L}$ . Use the attainable region algorithm to find the reactor network that maximizes the selectivity of C from A.

- (b) Show that for a series of chemical reactions, the molar change in the dependent components ( $\Delta n_d$ ) can be evaluated through the formulation  $\Delta n_d = -A_d^{-1}A_i\Delta n_i$ , where subscript 'i' indicates independent components, subscript 'd' indicates dependent components and 'A' indicates the stoichiometric components.

9 + 3 = 12

### Group – D

6. (a) What type of distillation column (tray/packed) will you select for an operation which involves: (i) corrosive systems (ii) system involving low-pressure fluids (iii) High liquid/gas ratio
- (b) Mention four important factors which influence the selection of the type of dryer.
- (c) Explain how adsorption selectivity is controlled in zeolite adsorbents.

6 + 4 + 2 = 12

7. (a) "Structured packing is most suitable for column revamps" – Explain this statement.
- (b) Write a note on gas permeation using membranes.

5 + 7 = 12

**Group – E**

8. (a) "Scheduling of a chemical process always leads to a binary integer programming" – Whether the statement is either true or false? Justify your answer.
- (b) The owner of a machine shop planned to expand the shop through purchasing some new machines – lathe and press. It was estimated that each press purchase will increase profit by Rs. 1000 and each lathe will increase profit by Rs. 500 daily. The number of machines that could be purchased is limited by the cost of the machine and available floor space area (see below table). The owner has Rs. 10,00,000 and 18.6 m<sup>2</sup> floor space area. Using branch and bound method estimate the number of each machine could be purchase to maximize the profit.

Machine	Required floor area (m <sup>2</sup> )	Price(Rs.)
Press	1.4	45,000
Lathe	2.8	1,00,000

**3 + 9 = 12**

9. (a) What is the purpose of LP relaxation?
- (b) A chemical equipment manufacturing company is considering expansion by building a new factory in either Surat or Gurgaon, or perhaps in both the cities. It is also considered to build at most one new warehouse, but the choice of location is restricted to a city where a new factory is being built. The net present value of each of these alternatives is shown in the below table. The rightmost column gives the capital required (already included in the net present value) for the respective instruments, where the total capital available in Rs. 10 crores. Find out the feasible combination of alternatives that maximizes the total present value.

Decision number	Yes-or-No Question	Decision Variable	Net Present value (Rs. Crores)	Capital Required (Rs. Crores)
1	Build factory in Surat?	X <sub>1</sub>	9	6
2	Build factory in Gurgaon?	X <sub>2</sub>	5	3
3	Build warehouse in Surat?	X <sub>3</sub>	6	5
4	Build warehouse in Gurgaon?	X <sub>4</sub>	4	2
<b>Capital available</b>			<b>10</b>	

**10 + 2 = 12**

Department & Section	Submission Link
CHE	<a href="https://classroom.google.com/c/MTQxOTM5MjM4OTcy/a/MjY0MjQxMDY3OTMw/details">https://classroom.google.com/c/MTQxOTM5MjM4OTcy/a/MjY0MjQxMDY3OTMw/details</a>