

BIRLA INSTITUTE OF TECHNOLOGY & SCIENCE, PILANI, PILANI CAMPUS
CHEMICAL ENGINEERING DEPARTMENT
 Course Title: Process Design Principles - I (CHE F314)
Comprehensive Examination (Closed Book)

Marks: 70

Date: 07/12/23

Time: 105 mins

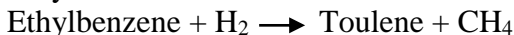
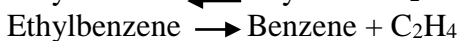
Note: Make suitable assumptions by clearly stating them, if necessary. Write all steps clearly.

1. (4+4 = 8 Marks)

- (a) In a mixture of two components, one component boils at a very low temperature (-75 °C) and the other component boils at 60 °C. If this mixture is separated in a distillation column, then would you prefer to operate this distillation column at atmospheric pressure or at higher pressure, and why?
- (b) Does the rule of thumb (heuristic), $L = 1.4 mG$, applicable for adiabatic operation in the absorber? If so, why? If not, why?

2. (15 Marks)

Styrene is produced from following reactions:



Product distribution data for styrene production are tabulated below in Table 1 and Table 2.

Table 1. Moles of benzene per mole of styrene versus conversion

Mol benzene/mol styrene	0.005	0.010	0.020	0.030	0.060	0.100	0.140
Conversion, x	0.10	0.15	0.20	0.25	0.30	0.35	0.40

Table 2. Moles of toluene per mole of styrene versus conversion

Mol toluene/mol styrene	0.006	0.015	0.030	0.045	0.070	0.110	0.160
Conversion, x	0.10	0.15	0.20	0.25	0.30	0.35	0.40

Develop the correlation for Selectivity (moles of styrene produced per mole of ethylbenzene reacted) and Conversion (x) using the method of averages or the method of linear least squares.

3. (4 Marks)

Acetone ($\text{C}_3\text{H}_6\text{O}$) is produced by dehydrogenation of isopropanol (IPA). To produce 100 lbmol/hr of acetone which mode (**batch vs continuous**) of operation would you suggest as per the heuristic. Provide proper justification for your answer.

4. (8 Marks)

Methanol (CH_3OH) is produced by the hydrogenation of carbon monoxide in the gas phase reaction as given below:



Pure carbon monoxide is used as a feed stream, but the hydrogen stream contains 2% of methane. The reactions take place at a temperature 340 °C. The allowable temperature range for these reactions is 300 – 400 °C. Whether the reactor is operated adiabatically or isothermally? Justify your answer with calculations. If your answer is isothermal, then suggest the way by which isothermal conditions would be maintained. Consider 100 moles/h of methanol production and selectively as 0.8. The specific heats in J/mol K of $\text{CO} = 28.95$, $\text{H}_2 = 28.84$, $\text{CH}_3\text{OH} = 52.29$, $\text{CH}_4 = 34.31$, $\text{H}_2\text{O} = 33.46$. Consider the feed rate (per hour) to the reactor as 200 moles CO , 600 moles H_2 , 250 moles CH_4 . 1 Btu = 1055 J and 1 lb = 453.3 g.

5. (25 Marks)

For the problem given with minimum approach temperature difference, $\Delta T_{\min} = 10\text{ }^{\circ}\text{C}$, carry out the Energy Integration Analysis using Pinch Technology by determining the following:

- Hot end design.
- Cold end design.
- Heat exchanger network for the maximum energy recovery (MER).
- Identification of loops.
- Break only first loop as per heuristic and restore ΔT_{\min} as and when there is a violation.

Stream No	Condition	FC_p (kW/ $^{\circ}\text{C}$)	h (kW/m 2 $^{\circ}\text{C}$)	Source Temperature ($^{\circ}\text{C}$)	Target Temperature ($^{\circ}\text{C}$)
1	Hot	3	0.4	170	60
2	Hot	1.5	0.55	150	30
3	Cold	2	0.75	20	135
4	Cold	6	0.65	80	140

Pinch temperature is $85\text{ }^{\circ}\text{C}$ (based on average). The minimum hot and cold utility requirements are 140 and 60 kW respectively.

6. (5 Marks)

1000 moles/h of a liquid mixture stream containing four components (A, B, C and D) as the following details is to be separated by distillation.

Component	Relative Volatility	Composition (mole%)	Property
A	4.7	30	Non-corrosive
B	2.58	20	Non-corrosive
C	1.7	30	Corrosive
D	2.6	20	Non-corrosive

Utilize the heuristics of simple column sequencing to draw all possible alternatives of distillation train with reference to column sequencing. Provide the justification for your answer.

7. (5 Marks)

100 kmol/h of a reactor effluent stream containing five components:

Component	Composition (mole%)	Boiling Point	Equilibrium Constant (K_i)	Nature
A	1	$-60\text{ }^{\circ}\text{C}$	100	Hydrocarbon
B	20	$-20\text{ }^{\circ}\text{C}$	0.002	Hydrocarbon
C	5	$10\text{ }^{\circ}\text{C}$	0.05	Volatile
D	30	$35\text{ }^{\circ}\text{C}$	0.001	Volatile
E	0.5	$-100\text{ }^{\circ}\text{C}$	150	Hydrocarbon
F	43.5	$5\text{ }^{\circ}\text{C}$	0.0005	Volatile

Based on the above-mentioned conditions, make the following decisions as per the conceptual design of process synthesis:

- Do we use phase split? Justify your answer.
- Do we use a vapor recovery system?
- Are any light ends present? If yes, then what would be the destination?

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Marks: 50

Date: 07/12/23

Time: 75 mins

Note: Make suitable assumptions by clearly stating them, if necessary. Write all steps clearly.

1. (35 Marks)

The production of allyl alcohol was developed partly for the purpose of producing epichlorohydrin via allyl alcohol as the intermediate, using a palladium catalyst.



In the first step of the process, the acetoxylation of propylene (pure) is carried out in the gas phase using oxygen (98% O₂ and 2% N₂), in the presence of a solid catalyst containing palladium as the main catalyst at 160 to 180°C and 70 to 140 psi. The reactor effluents from the reactor are separated into liquid components and gas components. The liquid components containing allyl acetate are sent to the hydrolysis process. The gas components contain unreacted gases and carbon dioxide and, after complete removal of the carbon dioxide, the unreacted gases are recycled to the reactor. In the second step, hydrolysis, which is an equilibrium reaction of allyl acetate, an acid catalyst is used and the reaction takes place at 60 to 80°C and allyl alcohol is selectively produced in almost 100% yield. Acetic acid recovered from the hydrolysis process, is reused in the first step.

Data Given:

Propylene: M.W. = 42 and B.P. = -46.6°C, Acetic Acid: M.W. = 60 and B.P. = 117.9°C, CO₂: M.W. = 44 and B.P. = -78.46°C, Allyl Acetate: M.W. = 100 and B.P. = 103°C, Allyl Alcohol: M.W. = 58 and B.P. = 97°C.

Cost Data: O₂ feed: Rs. 0.01/mole; C₃H₆: Rs. 2/kg; Acetic Acid: Rs. 10/kg; Allyl Alcohol: Rs. 15/kg; allyl acetate: Rs. 10/kg.

Selectivity is defined as the ratio of the number of moles of allyl alcohol produced to the number of moles of acetic acid reacted.

Based on the above-mentioned process and conditions, make the following decisions **with proper justification** as per the conceptual design of process synthesis (make suitable assumptions, if necessary):

- (a) Do we need to purify the feed streams before they enter the process?
- (b) How many product streams will be there?
- (c) How many reactor systems are required?
- (d) How many recycle streams are required?
- (e) Do we need to use an excess of any one reactant at the reactor inlet?
- (f) Assume the desired production rate for allyl alcohol is 250 mol/h, draw the input-output structure, and estimate the EP₂ in terms of design variable.
- (g) Draw the recycle structure of the flow sheet. Calculate the stream flow rates (recycle flows and reactor inlet) in terms of design variables.

Note: No marks will be given without appropriate justification.

2. (15 Marks)

Consider a very oversimplified design problem where the process consists only of a reactor, where two reactions $A_1 \rightarrow B_1$ and $A_2 \rightarrow B_2$ take place. The costs of the raw materials are C_{f1} and C_{f2} ; the desired production rates of B_1 and B_2 are P_1 and P_2 mol/hr respectively. Both reactions are first-order, isothermal, and irreversible with reaction rate constants k_1 and k_2 ; the densities are ρ_1 and ρ_2 ; the reactor downtimes are t_{d1} and t_{d2} ; the number of batches per year is n_1 and n_2 ; and only one reactor is used to make both products. Write the cost model with raw material and reactor costs for the total annual cost (TAC). How do the results for using two separate reactors compare to the results for using a single reactor for a case where the reactor cost is given by the following expression?

$$\text{Reactor cost} = C_v V^b; \quad b < 1$$

Where, C_v is cost per unit volume of the reactor (constant), b is constant and V is the volume of the reactor

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