**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**

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**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 $^oC$) and the other component boils at 60 $^oC$. 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:

   Ethylbenzene $\rightleftarrows$ Styrene + $H_2$
   Ethylbenzene $\longrightarrow$ Benzene + $C_2H_4$
   Ethylbenzene + $H_2$ $\longrightarrow$ Toulene + $CH_4$

   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 ($C_3H_6O$) 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:

$$CO + 2H_2 \rightarrow CH_3OH \qquad \Delta H_R = -104.69 \text{ kJ/mol}$$

$$CO + 3H_2 \rightarrow CH_4 + H_2O \qquad \Delta H_R = -198.28 \text{ kJ/mol}$$

   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 $^oC$. The allowable temperature range for these reactions is 300 – 400 $^oC$. 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 CO = 28.95, $H_2$ = 28.84, $CH_3OH$ = 52.29, $CH_4$ = 34.31, $H_2O$ = 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 °C, carry out the Energy Integration Analysis using Pinch Technology by determining the following:
(a) Hot end design.
(b) Cold end design.
(c) Heat exchanger network for the maximum energy recovery (MER).
(d) Identification of loops.
(e) Break only first loop as per heuristic and restore $\Delta T_{min}$ as and when there is a violation.

| **Stream No** | **Condition** | **$FC_p$ (kW/°C)** | **$h$ (kW/m$^2$ °C)** | **Source Temperature (°C)** | **Target Temperature (°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 °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 °C | 100 | Hydrocarbon |
| B | 20 | -20 °C | 0.002 | Hydrocarbon |
| C | 5 | 10 °C | 0.05 | Volatile |
| D | 30 | 35 °C | 0.001 | Volatile |
| E | 0.5 | -100 °C | 150 | Hydrocarbon |
| F | 43.5 | 5 °C | 0.0005 | Volatile |

Based on the above-mentioned conditions, make the following decisions as per the conceptual design of process synthesis:
(a) Do we use phase split? Justify your answer.
(b) Do we use a vapor recovery system?
(c) 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**

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**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.

$CH_3CH{=}CH_2$ + $CH_3COOH$ (Acetic Acid) + $O_2$ → $CH_2{=}CHOCOCH_3$ + $CO_2$

$CH_2{=}CHOCOCH_3$ + H2O → $CH_2{=}CHCH_2OH$ + $CH_3COOH$

In the first step of the process, the acetoxylation of propylene (pure) is carried out in the gas phase using oxygen (98% $O_2$ and 2% $N_2$), in the presence of a solid catalyst containing palladium as the main catalyst at 160 to 180$^o$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$^o$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$^o$C, Acetic Acid: M.W. = 60 and B.P. = 117.9$^o$C, $CO_2$: M.W. = 44 and B.P. = -78.46$^o$C, Allyl Acetate: M.W. = 100 and B.P. = 103$^o$C, Allyl Alcohol: M.W. = 58 and B.P. = 97$^o$C.

Cost Data: $O_2$ feed: Rs. 0.01/mole; $C_3H_6$: 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 $EP_2$ 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 $\rho_1$ and $\rho_2$; 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?

Reactor cost = $C_v V^b$;  $b < 1$

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

**ALL THE BEST**