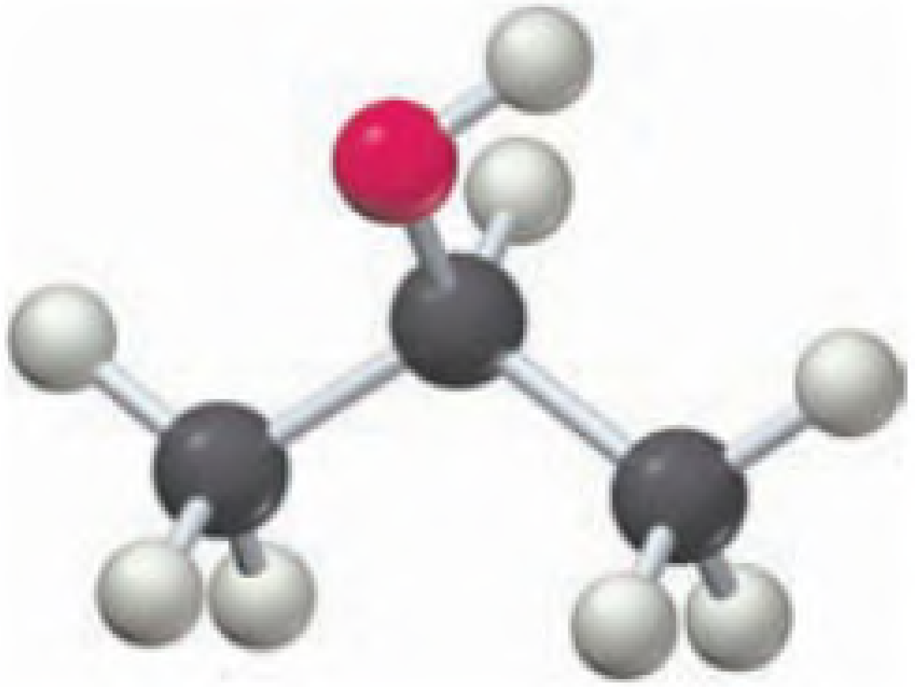
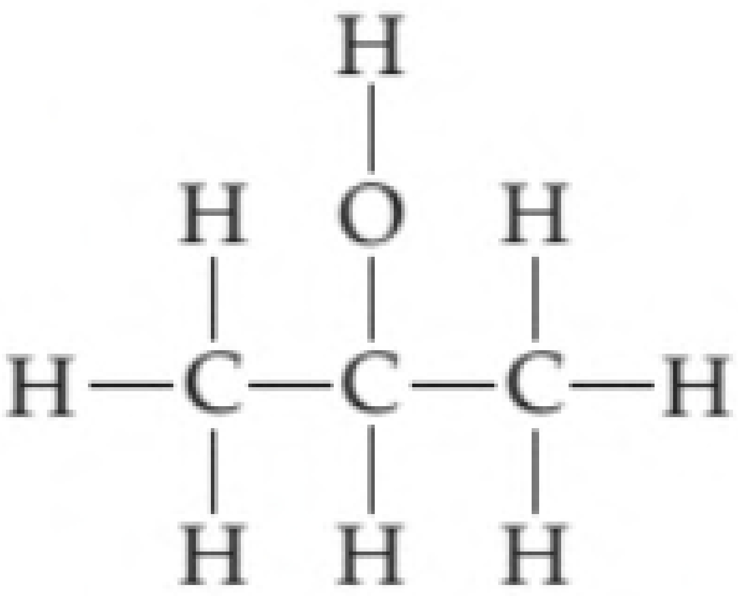
Comparison of Two Processes for Production of IPA





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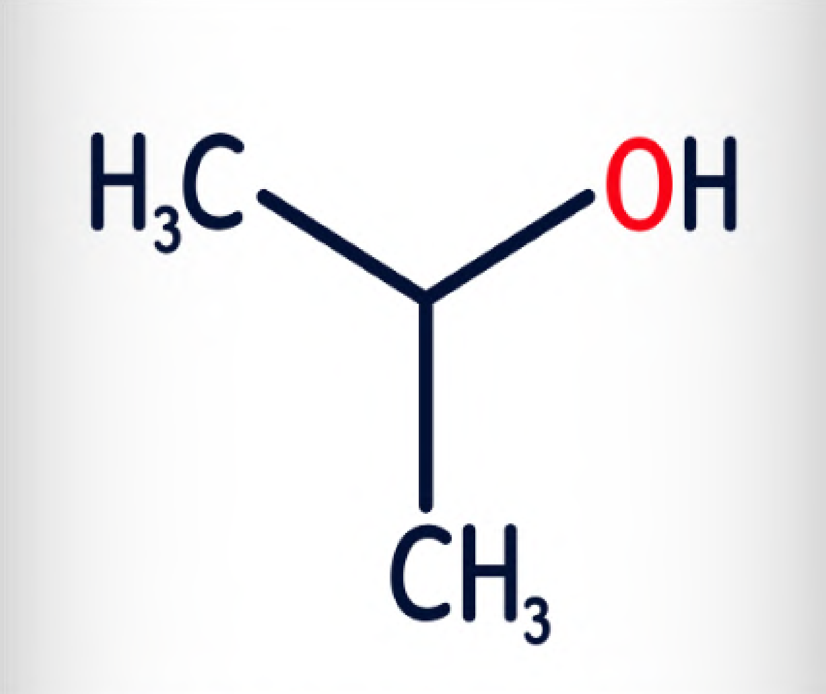
Description of the Project

The project focuses on the preparation of isopropyl alcohol (IPA), a secondary alcohol with the molecular formula C_3H_8O, which is widely used in industries such as pharmaceuticals, cosmetics and as a general-purpose solvent.



Isopropyl alcohol

Description of the Project

Two main methods are analyzed for producing IPA:

- **Direct Hydration (Tokuyama Process):** Acid-catalyzed direct hydration of propylene, producing high-purity IPA.

- **Indirect Hydration:** A two-step process involving the reaction of propylene with sulfuric acid, followed by hydrolysis producing IPA and sulfuric acid.

OBJECTIVES

1. Main objective of this project is to identify the most optimal process for manufacturing of isopropyl alcohol out of these two.

2. To simulate the most efficient process and do its enegy balance and identifying how minor changes like changing no. of distillation columns can change the efficiency.

3. Calculate the approx. cost for production of IPA in the efficient process.

Methodology

Two Production Methods for IPA:

1. Direct Hydration: Propylene is directly hydrated with water in the presence of an acidic catalyst.

2. Indirect Hydration: A two-step reaction involving sulfuric acid to form isopropyl sulfate, followed by hydrolysis to produce IPA.

Comparison:

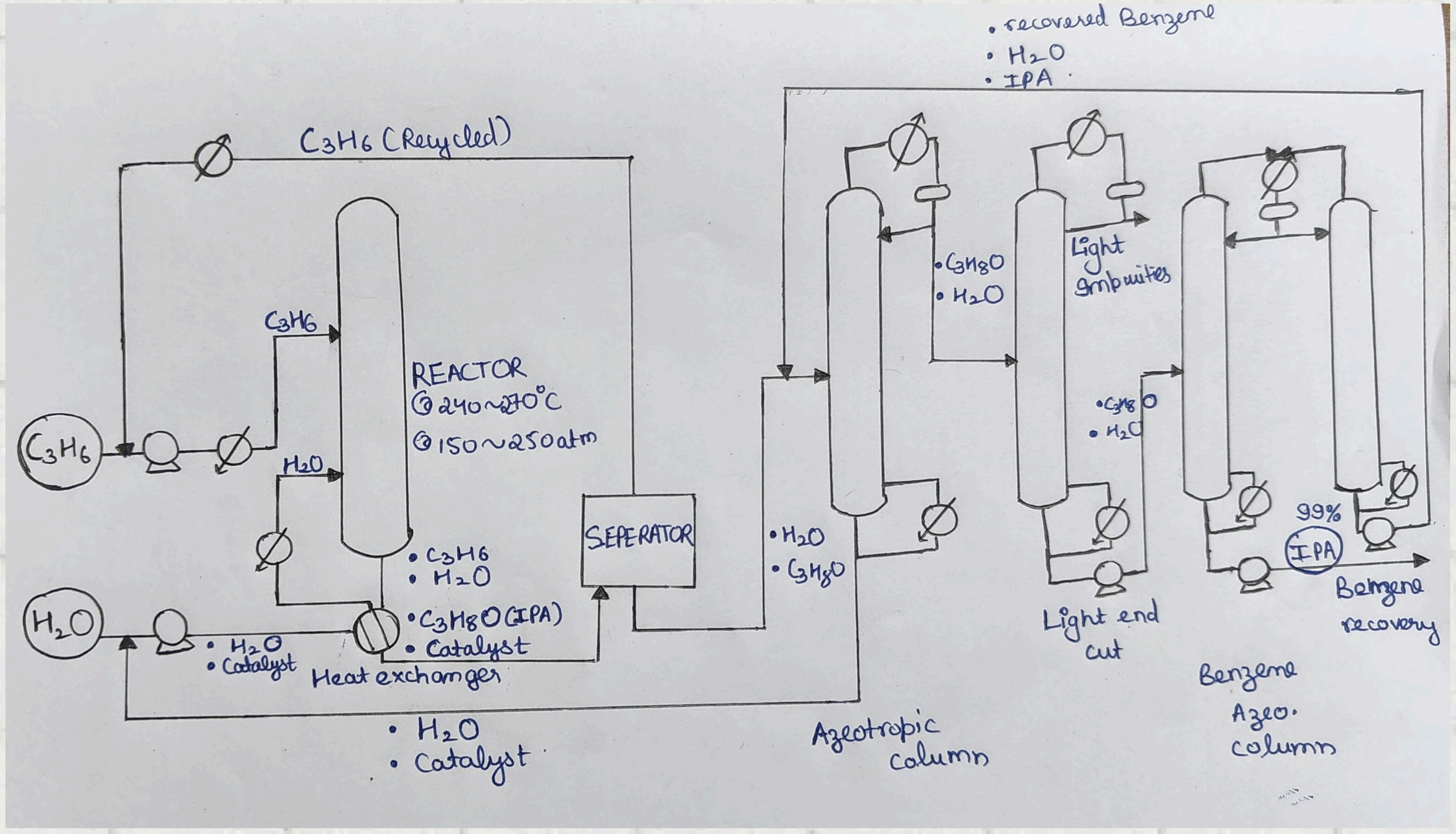
- **Direct Hydration** produces high-purity IPA with minimal by-products, making it a simpler, more efficient process.
- **Indirect Hydration** involves multiple chemical steps, increasing the formation of by-products like isopropyl ether, which requires additional separation steps.

DIRECT HYDRATION(TOKUYAMA PROCESS)

Reaction Equation:

$$CH_3-CH=CH_2+H_2O \xrightarrow{H^+} CH_3-\underset{\underset{}{}}{\overset{\overset{\displaystyle OH}{|}}{C}}H-CH_3$$

Propene — Isopropyl Alcohol



Flow Diagram of Tokuyama Process

Process Details:

- **Reaction:** Propylene reacts with water in the presence of a polytungsten catalyst.
- **Conditions:** High temperature (523 K) and pressure (50 - 60 atm) to ensure efficient conversion.

Advantages:

- The amount of unconverted propylene to be recycled is small owing to high conversion rate of propylene, and consequently this process does not require highly concentrated propylene feed.
- Higher yield of IPA with fewer separation requirements.
- The process is simple. It is also a completely closed system free from waste substances, and consequently the process can clear all the environmental protective regulation

INDIRECT HYDRATION

Process Steps:

1. Esterification: Propylene reacts with sulfuric acid, forming isopropyl hydrogen sulfate and di-isopropyl sulfate.

• Reaction: $CH3CH{=}CH2 + H2SO4 \leftrightharpoons (CH3)2CHOSO3H$

$$(CH_3)_2CHOSO_3H + CH_3CH{=}CH_2 \leftrightharpoons ((CH_3)_2CHO)_2SO_2$$

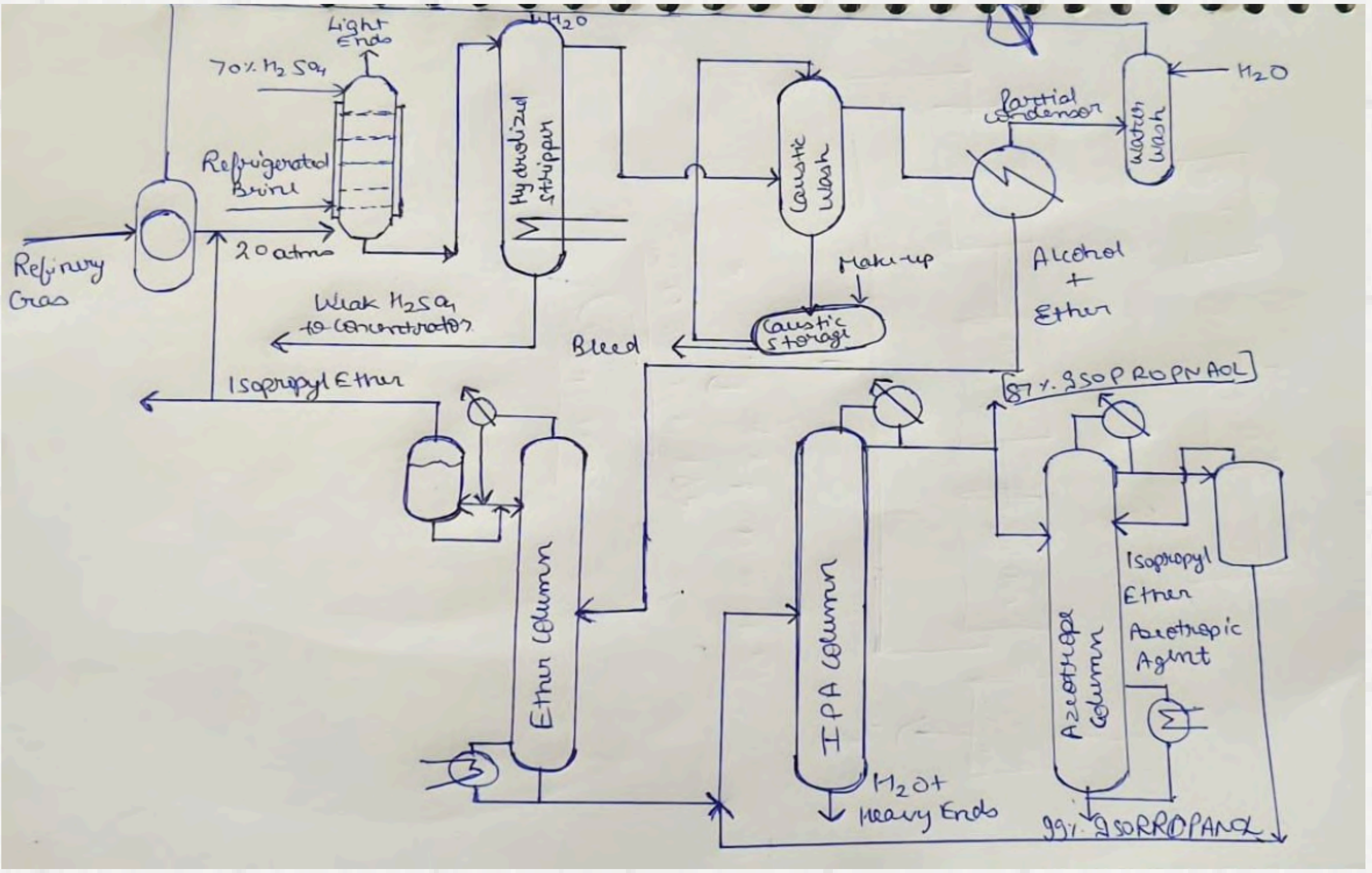
2. Hydrolysis: Isopropyl hydrogen sulfate is then hydrolyzed to produce IPA and regenerate sulfuric acid.

• Reaction: $(CH_3)_2CHOSO_3H + H_2O \leftrightharpoons (CH_3)_2CHOH + H_2SO_4$

Challenges with Indirect Hydration:

• Multi-step process introduces by-products such as isopropyl ether, reducing effective IPA yield.

• Sulfuric acid requirement and regeneration add to operating complexity and costs.



Flow Diagram of Indirect Process

MATERIAL BALANCE

To determine the material flow rates for reactants and products across each stage of reaction, ensuring optimal production and purity of IPA.

DIRECT HYDRATION MATERIAL BALANCE:

Feed and Reactor Balance:

- **Initial Feed:**
  - Propylene (C_3H_6): 34.967 kmol/hr
  - Water (H_2O): 49.9529 kmol/hr
- **Reactor Conversion:**
  - Single-pass conversion: 70%
  - Isopropyl alcohol (IPA) formed:34.967 kmol/hr.
  - Unreacted propylene is recycled back to the reactor , enhancing efficiency and yield.

Material Flow Across Reactor:

- **Total Material Entering:** 99.9058 kmol/hr

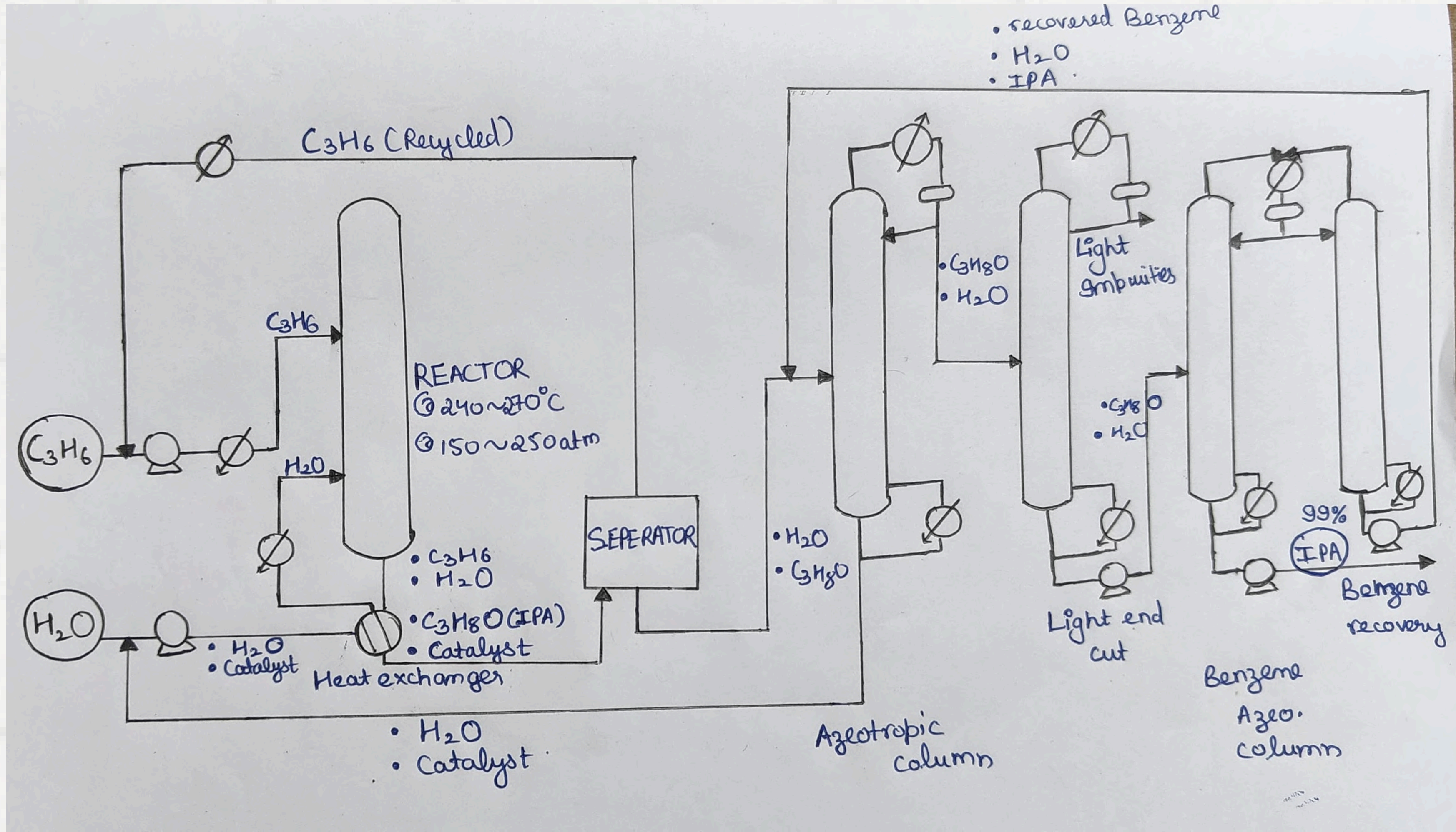
  Propylene: 49.9529 kmol/hr

  Water: 49.9529 kmol/hr
- **Material Leaving:**

  Isopropyl alcohol (IPA): 34.967 kmol/hr

  Unreacted water: 14.9859 kmol/hr
- **Efficiency:**

  Minimal waste as unreacted propylene is recycled



DIRECT HYDRATION MATERIAL BALANCE:

Material Flow Across Separator:

- **Total Material Entering:** 64.9388 kmol/hr
  Propylene: 14.9859 kmol/hr
  Water: 14.9859 kmol/hr
  Isopropyl alcohol: 34.967 kmol/hr
- **Material Leaving:**
  Isopropyl alcohol (IPA): 34.967 kmol/hr
  Unreacted water: 14.9859 kmol/hr
  Recycled Propylene: 14.9859 kmol/hr

Across Distillation columns:

- **Total material Entering:**
  - 49.9529 kmol/hr
  - Isopropyl Alcohol: 34.967 kmol/hr
  - Water:14.9859 kmol/hr
- **Total Material leaving:**
  <u>Top stream</u>:
    - Isopropyl alcohol: 34.9382 kmol/hr
    - Water: 0.028769 kmol/hr

  <u>Bottom stream</u>:
    - Water: 14.9571 kmol/hr
    - Isopropyl Alcohol: 0.0287698 kmol/hr

DIRECT HYDRATION MATERIAL BALANCE:

	Units	C2H6	H2O	C2H6+H20	PRODUCT	HEP	RECYC3H6	IPA+H2O	TOP1	BOT1	TOP2	BOT2	TOP3
Average MW		42.0806	18.0153	30.048	46.2276	46.2276	42.0806	47.4717	48.0445	18.0154	50.7138	18.0154	54.801
− Mole Flows	**kmol/hr**	**34.967**	**49.9529**	**99.9058**	**64.9388**	**64.9388**	**14.9859**	**49.9529**	**49**	**0.9529**	**45**	**4**	**4**
PROPY-01	kmol/hr	34.967	0	49.9529	14.9859	14.9859	14.9859	0	0	0	0	0	
ISOPR-01	kmol/hr	0	0	0	34.967	34.967	0	34.967	34.967	1.64375e-06	34.967	1.15414e-05	34.96
WATER	kmol/hr	0	49.9529	49.9529	14.9859	14.9859	0	14.9859	14.033	0.952898	10.033	3.99999	5.0330
BENZENE	kmol/hr	0	0	0	0	0	0	0	0	0	0	0	
− Mole Fractions													
PROPY-01		1	0	0.5	0.230769	0.230769	1	0	0	0	0	0	
ISOPR-01		0	0	0	0.538461	0.538461	0	0.699999	0.713612	1.725e-06	0.777044	2.88536e-06	0.87417
WATER		0	1	0.5	0.23077	0.23077	0	0.300001	0.286388	0.999998	0.222956	0.999997	0.12582
BENZENE		0	0	0	0	0	0	0	0	0	0	0	
− Mass Flows	**kg/hr**	**1471.43**	**899.915**	**3001.96**	**3001.96**	**3001.96**	**630.614**	**2371.35**	**2354.18**	**17.1668**	**2282.12**	**72.0616**	**2192.0**
PROPY-01	kg/hr	1471.43	0	2102.05	630.614	630.614	630.614	0	0	0	0	0	
ISOPR-01	kg/hr	0	0	0	2101.37	2101.37	0	2101.37	2101.37	9.87829e-05	2101.37	0.000693593	2101.3
WATER	kg/hr	0	899.915	899.915	269.975	269.975	0	269.975	252.808	17.1667	180.748	72.0609	90.671
BENZENE	kg/hr	0	0	0	0	0	0	0	0	0	0	0	
− Mass Fractions													
PROPY-01		1	0	0.700224	0.210067	0.210067	1	0	0	0	0	0	
ISOPR-01		0	0	0	0.7	0.7	0	0.886151	0.892613	5.75429e-06	0.920798	9.62499e-06	0.95863
WATER		0	1	0.299776	0.0899329	0.0899329	0	0.113849	0.107387	0.999994	0.0792016	0.99999	0.041363
BENZENE		0	0	0	0	0	0	0	0	0	0	0	
Volume Flow	l/min	24819	35455.8	66399.7	189.946	6040.21	6499.83	49.8192	53.4767	0.311579	52.1688	1.30792	50.5
+ Vapor Phase													

DIRECT HYDRATION MATERIAL BALANCE:

Material | Heat | Load | Work | Power | Vol.% Curves | Wt. % Curves | Petroleum | Polymers | Solids

	Units	YC3H6	IPA+H2O	TOP1	BOT1	TOP2	BOT2	TOP3	BOT3	BOT4	MIX	FINALBOT	FINALIPA
Average MW		42.0806	47.4717	48.0445	18.0154	50.7138	18.0154	54.8011	18.0155	18.2555	18.0154	18.0961	60.0613
− Mole Flows	**kmol/hr**	**14.9859**	**49.9529**	**49**	**0.9529**	**45**	**4**	**40**	**5**	**5.033**	**9.9529**	**14.9859**	**34.967**
PROPY-01	kmol/hr	14.9859	0	0	0	0	0	0	0	0	0	0	0
ISOPR-01	kmol/hr	0	34.967	34.967	1.64375e-06	34.967	1.15414e-05	34.967	2.32828e-05	0.0287324	3.64679e-05	0.0287689	34.9382
WATER	kmol/hr	0	14.9859	14.033	0.952898	10.033	3.99999	5.03304	4.99998	5.00427	9.95286	14.9571	0.028769
BENZENE	kmol/hr	0	0	0	0	0	0	0	0	0	0	0	0
− Mole Fractions													
PROPY-01		1	0	0	0	0	0	0	0	0	0	0	0
ISOPR-01		0	0.699999	0.713612	1.725e-06	0.777044	2.88536e-06	0.874174	4.65655e-06	0.00570881	3.66405e-06	0.00191973	0.999177
WATER		0	0.300001	0.286388	0.999998	0.222956	0.999997	0.125826	0.999995	0.994291	0.999996	0.99808	0.000822747
BENZENE		0	0	0	0	0	0	0	0	0	0	0	0
− Mass Flows	**kg/hr**	**630.614**	**2371.35**	**2354.18**	**17.1668**	**2282.12**	**72.0616**	**2192.04**	**90.0774**	**91.88**	**179.306**	**271.186**	**2100.16**
PROPY-01	kg/hr	630.614	0	0	0	0	0	0	0	0	0	0	0
ISOPR-01	kg/hr	0	2101.37	2101.37	9.87829e-05	2101.37	0.000693593	2101.37	0.0013992	1.7267	0.00219157	1.72889	2099.65
WATER	kg/hr	0	269.975	252.808	17.1667	180.748	72.0609	90.6716	90.076	90.1533	179.304	269.457	0.518281
BENZENE	kg/hr	0	0	0	0	0	0	0	0	0	0	0	0
− Mass Fractions													
PROPY-01		1	0	0	0	0	0	0	0	0	0	0	0
ISOPR-01		0	0.886151	0.892613	5.75429e-06	0.920798	9.62499e-06	0.958636	1.55333e-05	0.018793	1.22226e-05	0.00637531	0.999753
WATER		0	0.113849	0.107387	0.999994	0.0792016	0.99999	0.0413639	0.999984	0.981207	0.999988	0.993625	0.000246781
BENZENE		0	0	0	0	0	0	0	0	0	0	0	0

INDIRECT HYDRATION MATERIAL BALANCE:

Initial Feed:

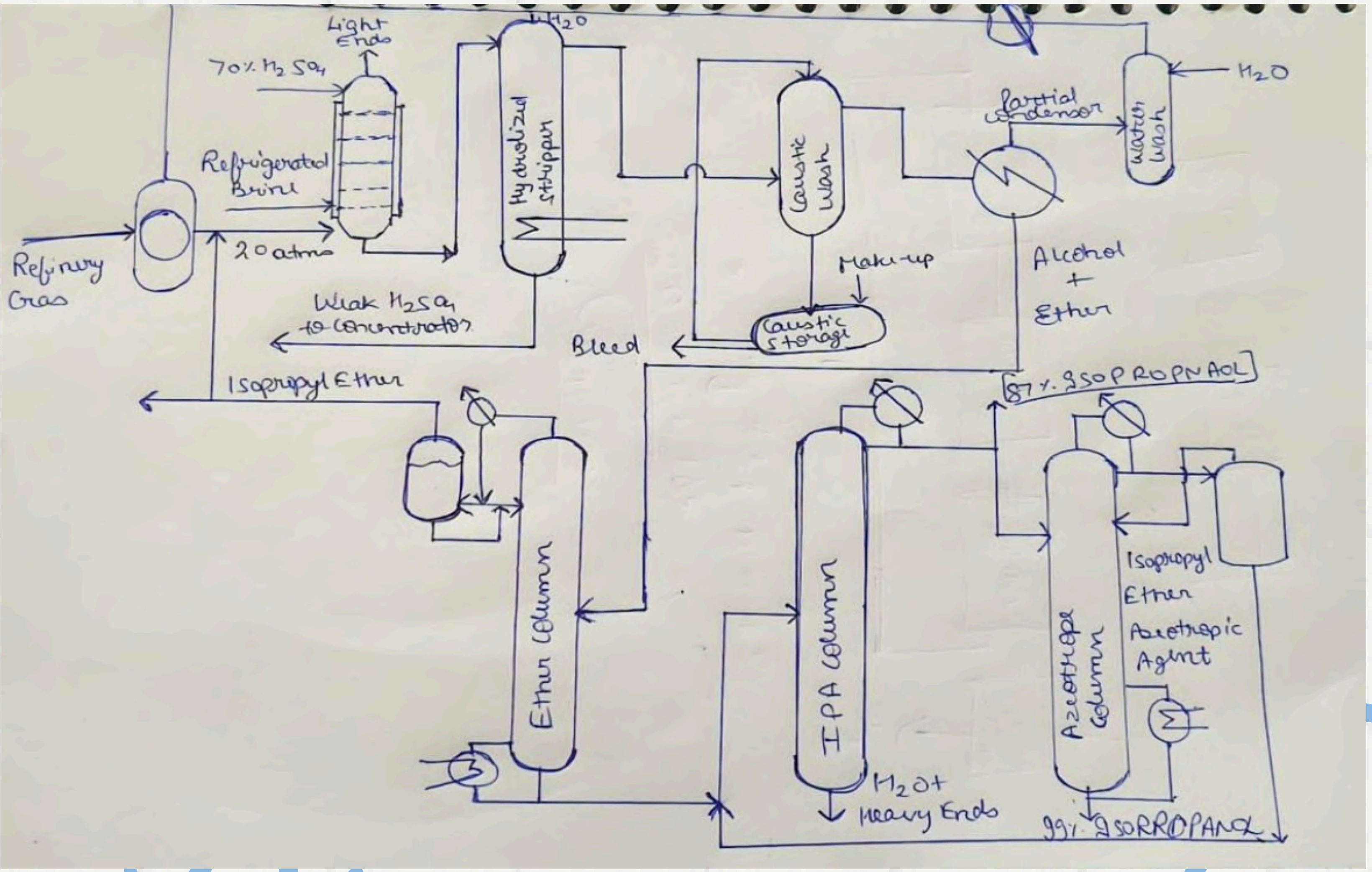
- Propylene: 34.967 kmol/hr
- Sulfuric acid: Adjusted based on reaction needs (70% concentration).

Absorber Conversion:

- 70% of propylene reacts, forming isopropyl sulfate.

Hydrolyser Balance:

- Input: Isopropyl sulfate and water
- Output: IPA - 24.477 kmol/hr



Balance across Ether Column:

- Let's assume that 1% of IPA is converted to isopropyl ether during the separation
- Remaining Isopropanol: 24.477 kmol/hr * 0.99 = 24.232 kmol/hr.
- OUTPUT : (a) Isopropyl Ether: 0.245 kmol/hr (b) Isopropanol: 24.232 kmol/hr (goes to the IPA column).

Balance Across the IPA Column:

In the IPA column, the feed is separated into 87% isopropanol and 13% water.

1) Feed to IPA Column:

- Isopropanol: 24.232 kmol/hr.
- Water Content: Assume it's negligible initially.

2) Separation Products:

- 87% Isopropanol (IPA) Mixture: 24.232 kmol/hr * 0.87 = 21.080 kmol/hr.
- Water Content: 24.232 kmol/hr * 0.13 = 3.152 kmol/hr.

3) Output:

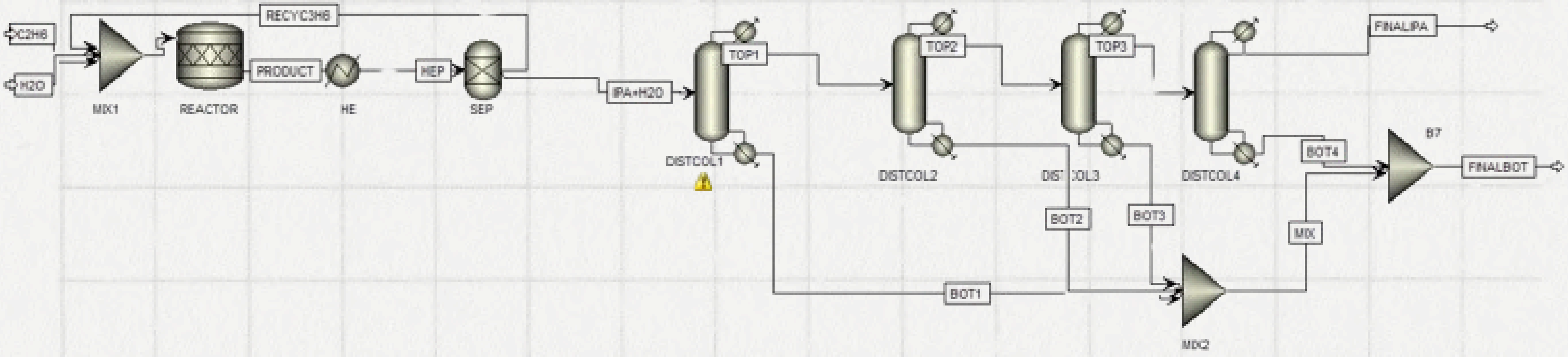
- 87% IPA Mixture: 21.080 kmol/hr, goes to the azeotropic distillation column.
- Water and Waste: 3.152 kmol/hr, removed from the system.

By-products:

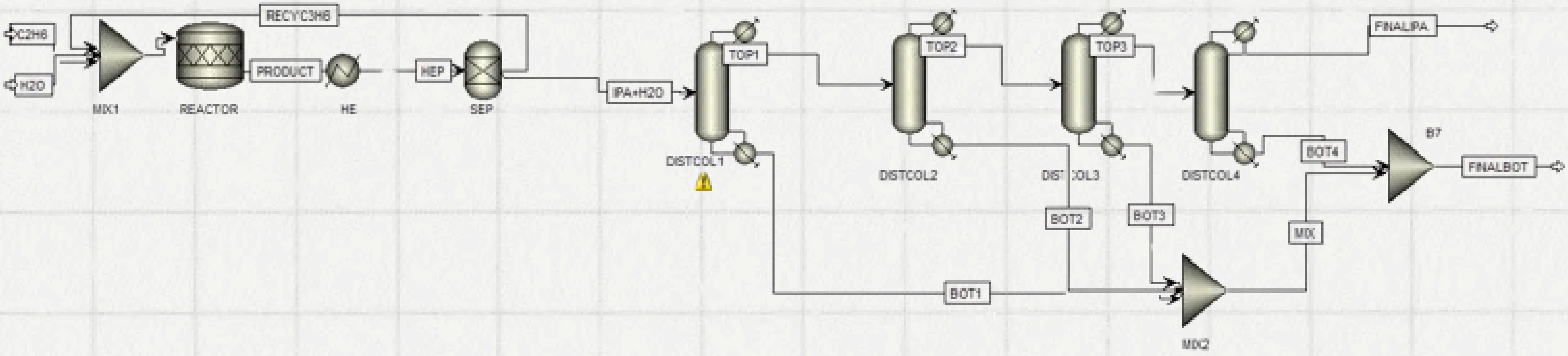
- Unreacted propylene, minimal acidic impurities, and isopropyl ether reduce IPA yield compared to Direct Hydration.

IN SHORT

- We have taken same amount of Propylene in both methods i.e.34.967Kmol/hr. But the final Output in direct hydration method is more (IPA=34.967 Kmol/hr) compared to indirect hydration method (IPA=21.080 Kmol/hr).
- So, from this we can conclude that Efficiency of Direct Hydration method is more than efficiency of Indirect Hydration method.
- Some notable's reasons can be as Indirect method involves multiple chemical steps (sulfonation, hydrolysis, caustic neutralization) that generate intermediate compounds, which reduces the effective yield of IPA.
- In Direct Hydration method, minimal by-products are formed, the primary reaction results in IPA, and any unreacted propylene is typically recycled. This means there is little to no generation of undesirable compounds, leading to higher product yield and less waste.
- Whereas in Indirect Hydration method, the formation of by-products like isopropyl ether and unreacted isopropyl sulphate, which must be separated and either discarded or recycled.
- These unwanted By-products reduce the amount of available IPA in each cycle, effectively lowering the yield per unit of propylene and making the process less efficient overall.

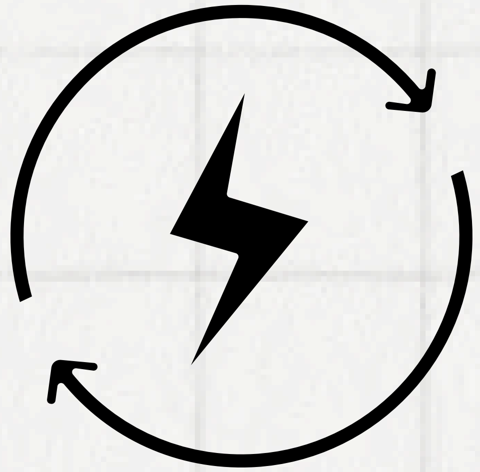


- A stoichiometric conversion reactor receives a feed of C3H6 and H_2O, both at 519 K, where the desired reaction takes place.
- The product stream exiting the reactor at 523 K is passed through a heat exchanger to cool the gases down to 313 K.
- In the next step, C3H6 is separated and recycled from the product stream, while the remaining mixture of IPA and water is sent to a distillation setup.
- For the distillation process, a 30-stage column is used with a feed plate positioned at the 12th stage and a reflux ratio of 2.6, optimized to maximize the IPA concentration in the distillate



- Testing with multiple distillation columns showed the following IPA purities in the distillate:
- 99.72% with a single column,
- 99.78% with two columns,
- 99.83% with three columns, and
- 99.91% with four columns.
- The increase in purity slowed significantly with each additional column and using five columns offered minimal additional benefit. Therefore, we chose to implement four distillation columns, balancing the high IPA purity with the cost-effectiveness of the setup.

ENERGY BALANCE



Energy balances are made to determine the energy requirements of the process.

The steady state energy balance calculated using relation:
Energy out = Energy in + Heat of reaction + Q(heat supplied/heat removed).

ENERGY BALANCE OF DIRECT HYDRATION PROCESS

The reference temperature is 273k and we have used :energy=n*specific heat*temp difference

Across Reactor

- Operating Conditions: The reactor operates at a temperature of 523 K and a pressure of 200 atm.
- Total Energy Entering the Reactor: 753.795 kJ/s.
- Total Energy Leaving the Reactor: 1132.24 kJ/s.

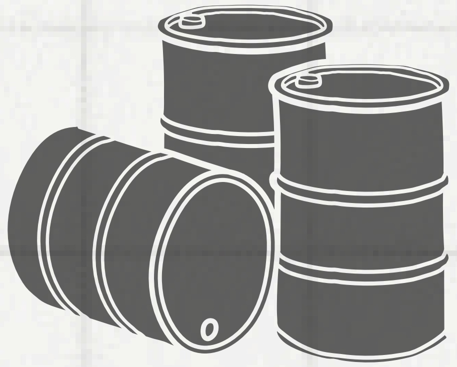
Heat Exchanger

- Cools the product stream to a temperature of 313 K
- Total Energy Entering .the Heat Exchanger:1144.15kJ/s
- Total Energy Leaving the Heat Exchanger: 236.27 kJ/s.

Condenser and Reboiler

- Condenser: Used to condense the vapor product, ensuring minimal energy loss.
- Reboiler: Provides the necessary heat input to maintain the separation process.
- Total energy changes calculated to optimize heat recovery in the process

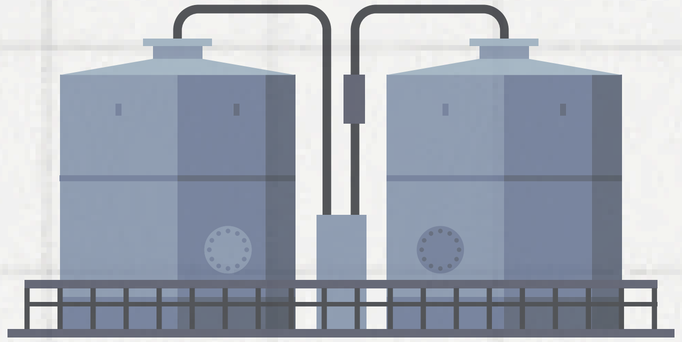
COST ANALYSIS



1. Raw Material Costs:

- Propylene: 3,671,535 INR/hr (34.967 kmol/hr required).
- Water: 17 INR/hr (34.967 kmol/hr required).
- Total Raw Material Cost: ~36 lakh INR/hr.

2. Equipment Costs:



- Reactor: ~1-1.5 Crore INR.
- Heat Exchanger: 12 Lakh INR.
- Separator: 10 Lakh INR.
- Distillation Columns (4): 68 Lakh INR each.
- Condensers and Reboilers: Included in setup costs.
- Total Equipment Cost: ~2.5 Crore INR.

3. Annual Operational Costs:

- Estimated operational cost: 14.75 Crore INR/year (excluding land, labor, and electrical equipment).

4. Profitability:

- Gross Income: 23.54 Crore INR/year.
- Net Profit After Taxes (30%): 17.39 Crore INR/year.

Thank you!

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