Comparison of Two Processes for Production of IPA

Group 14

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1)Description of the Project: The project focuses on the preparation of isopropyl alcohol (a secondary alcohol, with the molecular formula C_3H_8O), a vital chemical compound extensively used in various industries, including pharmaceuticals, cosmetics, and as a general-purpose solvent.
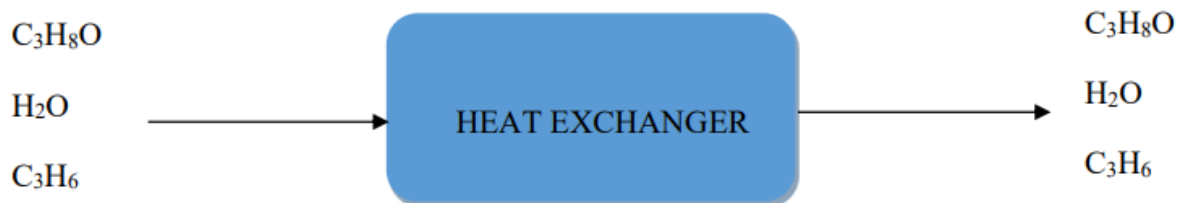
There are two ways to form it:

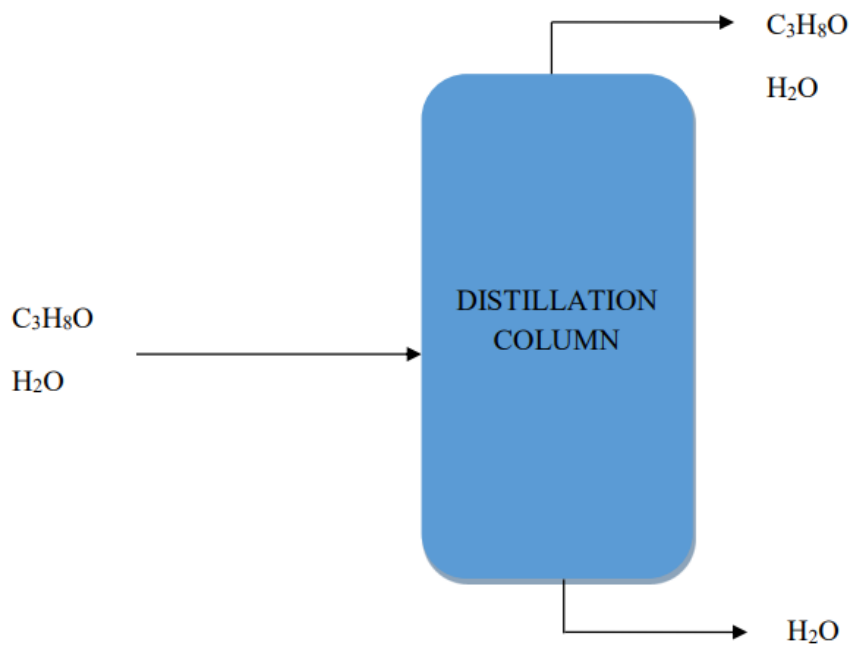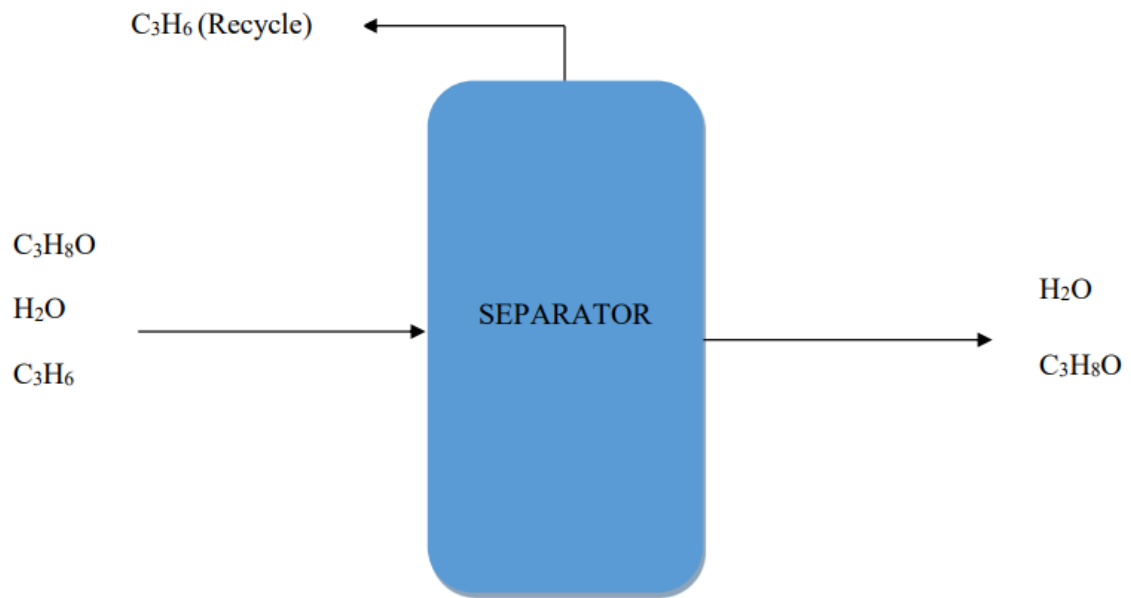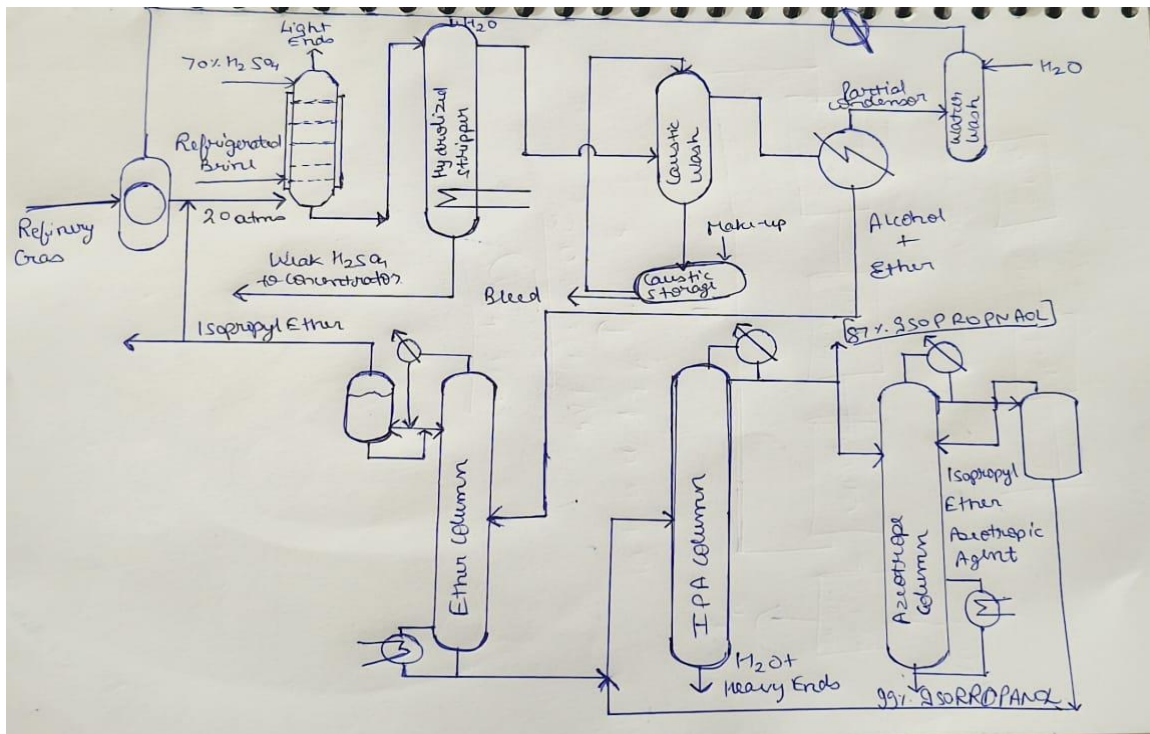a) Direct Hydration
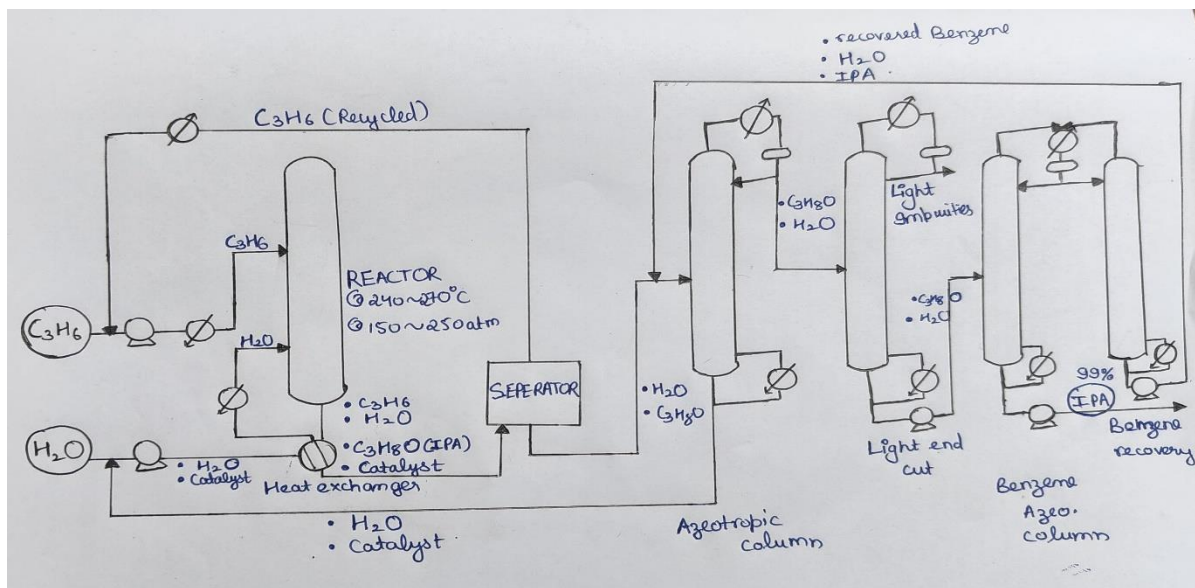
Flow Diagram for Tokuyama process

Broke the flowsheet in simpler components for material balance:

C₃H₆ (Recycle) ←

SEPARATOR

C₃H₈O
H₂O
C₃H₆
→

→ H₂O
C₃H₈O

DISTILLATION COLUMN

→ C₃H₈O
H₂O

C₃H₈O
H₂O
→

→ H₂O

b) Indirect Hydration

Flow Diagram for indirect hydration

References:

1. Kirk-Othmer encyclopaedia of chemical technology, fifth edition.
 2. https://www.statista.com/statistics/974791/us-isopropanol-production-volume/
3. http://isopropylalcohol.weebly.com/history.html
4. https://en.wikipedia.org/wiki/Isopropyl_alcohol

2)Objectives of the project:

  a) Our objective in this project is to identify the most optimal process for manufacturing of isopropyl alcohol out of these two.

  b) to check how changes in number of distillation columns would affect Tokuyama process.

  c) calculate the approx. cost for production of IPA in the efficient process.

3)Methodology:

 a) Direct Hydration: The acid-catalysed direct hydration of propylene is exothermic and resembles the preparation of ethyl alcohol from ethylene.

i) $CH_3CH_2=CH_2 + H_3O^+ \leftrightharpoons CH_3CH—CH_2 + H_2O$ fast

$$\searrow + \swarrow$$
$$H$$

ii) $CH_3CH—CH_2 \leftrightharpoons (CH_3CHCH_3)$ slow

$$\searrow + \swarrow$$
$$H$$

$$OH$$
$$|$$
iii) $CH_3CH^+CH_3 + 2H_2O \leftrightharpoons CH_3CHCH_3 + H_3O^+$ fast
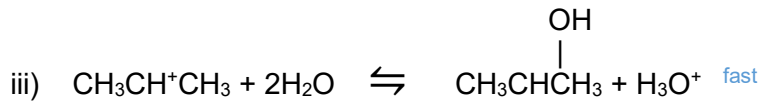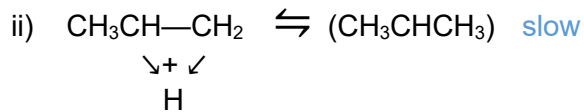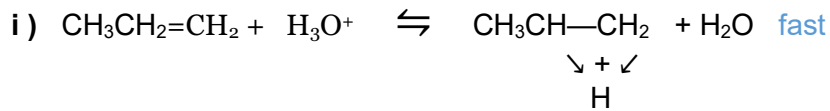
We will majorly use the <u>Tokuyama soda process (one of the processes used in direct hydration)</u> for our project:

The Tokuyama process is a variation of the direct hydration method used to produce isopropyl alcohol. In this process, propylene is directly hydrated with water in the presence of a highly acidic catalyst, typically phosphoric acid supported on a solid carrier. The reaction is carried out under high temperature and pressure conditions.

$$(CH_3)_2CHOSO_3H + 2H_2O \leftrightharpoons 2(CH_3)_2\,CHOH + H_2SO4$$
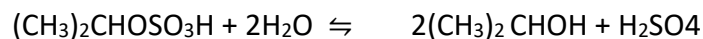
Material Balance:

Let's say in a plant 50 tonnes of Iso-propyl Alcohol is produced everyday

→ 34.967 kmol/hr also we require same amount of water moles

⟹ feed = 34.967 kmol/hr of IPA and water

<u>ACROSS REACTOR & SEPRATOR</u>

Fresh feed = 34.967 kmol/hr of IPA & H_2O

Single pass conversion of reactor is 70%

Therefore, Isopropyl formed = 0.7 × feed entering

feed → | **Reactor** | → | **Separator** | → C3H8O
                                              H2O
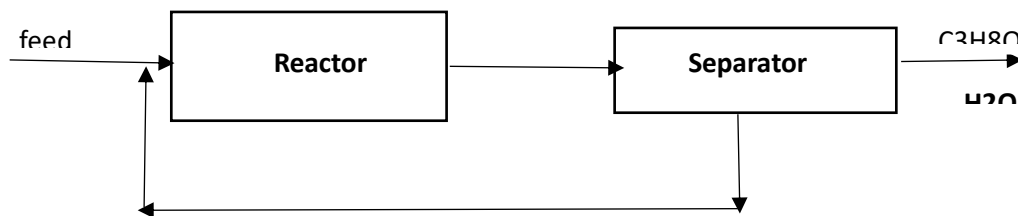
(Amount of C3H8O/amount of propylene) = 0.7
   ⟹ X = 49.9592 kmol/hr
∴ Water and propylene entering reactor = 49.9592 kmol/hr

<u>ACROSS DISTILLATION COLUMN</u>

C3H8O & **H2O** → [box] → **C3H8O** & **H2O**

H2O
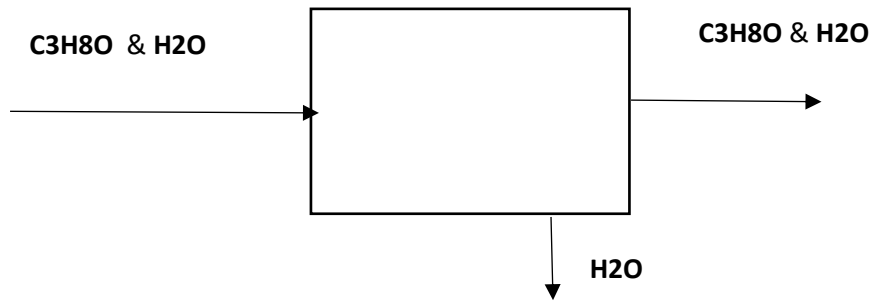
We need 99% pure IPA i.e. 1% water comes out with IPA

IPA entering = 34.967

H_2O entering = 14.9859

Top stream will contain 99% IPA

$\implies 0.99 \times 34.967 = 34.617$

Also, $0.01 \times 34.967 = 0.34967$ water

Material balance across reactor

Compounds	Material entering (kmol/h)	Inside reactor(kmol/h)	Material leaving(kmol/h)
Propylene	49.9529	-34.967	14.9859
Water	49.9529	-34.967	14.9859
Isopropyl alcohol	0	34.967	34.967
Total	99.9057	34.967	64.9387

Material balance across heat exchanger

Compounds	Material entering (kmol/h)	Material leaving(kmol/h)
Propylene	14.9859	14.9859
Water	14.9859	14.9859
Isopropyl alcohol	34.967	34.967
Total	64.9387	64.9387

Material balance across separator

Compounds	Material entering(kmol/h)	Recycle(kmol/h)	Material leaving(kmol/h)
Propylene	14.9859	14.9859	o

	14.9859	0	14.9859
Water	14.9859	0	14.9859
Isopropyl alcohol	34.967	0	34.967
Total	64.9387	14.9859	49.9528

Material balance across distillation column

Compounds	Material entering(kmol/h)	Top stream(kmol/h)	Material leaving(kmol/h)
Propylene	0	0	0
Water	14.9859	0.34967	14.6361
Isopropyl Alcohol	34.967	34.617	0.35
Total	49.9528	34.967	14.9861

Material balance across the entire process

Compounds	Material entering(kmol/h)	Material leaving(kmol/h)
Propylene	34.967	0
Water	49.9528	14.9859
Isopropyl Alcohol	0	34.967
Total	84.9198	49.9528

Energy Balance:

ACROSS REACTOR

From Separator C3H6

C3H6

H2O

REACTOR

C3H6

H2O

IPA
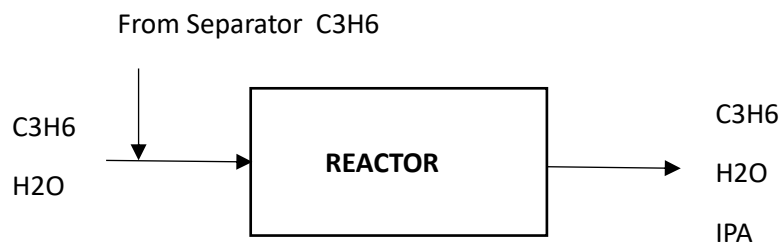
For an isentropic process, pressure-temperature relation is given by

P1= 1atm

P2= 200atm

R= 0.0821L.atm/K.mol

Cp= 84.5495

T2= 250° C

$$T2/T1 = (P2/P1)^{(R/Cp)}$$

$$T1 = (523) \times (1/200)^{(84.5495/0.0821)}$$

$$\implies T1= 246° C$$

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

	ENTERING				LEAVING			
	Mass flow rate (kmol/hr)	Specific heat (kJ/kmol K	T(K)	Energy (KJ/s)	Mass flow rate (kmol/hr)	Specific heat (kJ/kmol K)	T(K)	Energy (KJ/s)
C_3H_6	49.95286	131.0667	519	445.570	14.98586	131.733	523	137.0925
H_2O	49.95286	90.666	519	308.225	14.98586	90.666	523	95.4728
IPA	-	-	-	-	34.967	375.4043	523	899.6766
	TOTAL			753.795	TOTAL			1132.24

From energy balance equation,

Total Energy Leaving = Total Energy Entering

Energy Out = Energy In + Heat of Reaction + Q

Q=0 (since the process is adiabatic)

Heat of reaction=378.4521kJ/s

Heat exchanger:

C3H6
H2O
IPA

HEAT EXCHANGER

C3H6
H20
IPA

	ENTERING					LEAVING			
	Mass flow rate (kmol/hr)	Specific heat (kJ/kmol-K)	T(K)	Energy (kJ/s)		Mass flow rate (kmol/hr)	Specific heat (kJ/kmol-K)	T(K)	Energy (kJ/s)
C_3H_6	14.98586	131.733	523	137.0925		14.98586	103.733	313	158.0113
H_2O	14.98586	91.746	523	95.47866		10.4901	74.43	313	12.39331
IPA	34.967	375.4043	523	911.5827		34.967	169.5153	313	65.86046
	TOTAL			1144.152					236.2651

From energy balance equation,

Total Energy Leaving= Total Energy Entering

Energy Out = Energy In + Heat of Reaction + Q

236.2651=1144.152+0+Q

$\implies$ Q = -907.8869/s

Condenser:
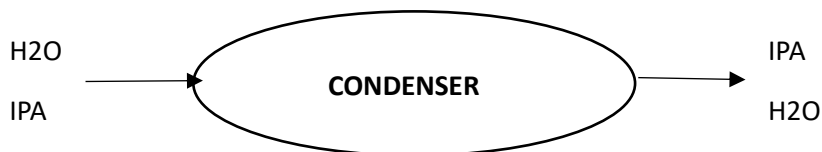
	Entering					Leaving			
	Mass flow rate (kmol/hr)	Specific heat (kJ/kmol-K)	T(K)	Energy (kJ/s)		Mass flow rate (kmol/hr)	Specific heat (kJ/kmol-K)	T(K)	Energy (kJ/s)
H2O	0.34967	75.6576	363	0.66137		0.34967	75.2661	323	0.21931
IPA	34.967	218.5365	363	191.0391		34.967	165.0554	323	48.0957
	Total			191.7005		TOTAL			48.31508

From energy balance equation,

Total Energy Leaving= Total Energy Entering

Energy Out = Energy In + Heat of Reaction + Q

48.31508 = 191.7005 + 0 + Q

$\implies$ Q = -143.385 kJ/s

Reboiler:
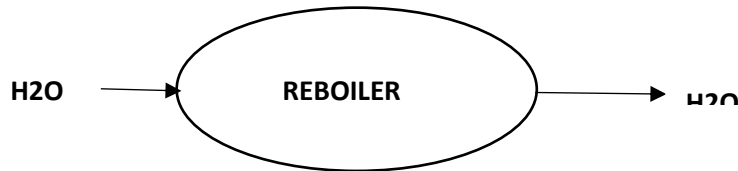
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  H2O  ──────▶  (  REBOILER  )  ──────▶  H2O
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	ENTERING					LEAVING			
	Mass flow rate (kmol/hr)	Specific Heat (kJ/kmol-K)	T(K)	Energy (kJ/s)		Mass flow rate (kmol/hr)	Specific Heat (kJ/kmol-K)	T(K)	Energy (kJ/s)
H2O	10.14043	75.312	333	12.72826		10.14043	75.7224	378	22.3958
	TOTAL			12.72826		TOTAL			22.3958

From energy balance equation,

Total Energy Leaving= Total Energy Entering

Energy Out = Energy In + Heat of Reaction + Q

22.3958 = 12.72826 + 0 + Q

$\implies$ Q = 9.6674 kJ/s

Reboiler duty = 9.6674 kW

b) **Indirect Hydration**: This process is based on a two-step reaction of propylene and sulfuric acid. In the first step, mixed sulphate esters, primarily isopropyl hydrogen sulphate, but also Di isopropyl sulphate, form. These are then hydrolysed, forming the alcohol and sulfuric acid.

Step 1. Esterification:

$$CH_3CH=CH_2 + H_2SO_4 \leftrightharpoons (CH_3)_2CHOSO_3H$$

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

Step 2. Hydrolysis:

$$(CH_3)_2CHOSO_3H + H_2O \leftrightharpoons (CH_3)_2CHOH + H_2SO_4$$

$$(CH_3)_2CHOSO_3H + 2H_2O \rightleftharpoons 2(CH_3)_2 CHOH + H_2SO4$$
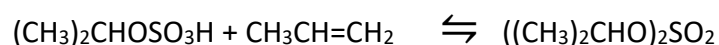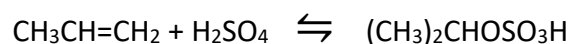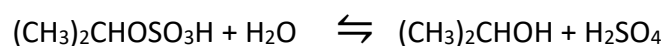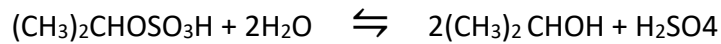
Material Balance (Indirect Hydration):

We have taken feed rate as 34.967 kmol/hr of propylene (C_3H_6) and 70% concentrated sulfuric acid (H_2SO_4). 70% single-paas conversion for propylene in the absorber.

First, we will do <u>material balance across the absorber column</u>.

The primary reaction in the absorber is the reaction of propylene with sulphuric acid to form isopropyl sulphate.

1. Feed to Absorber:

    a. Propylene (C_3H_6): 34.967 kmol/hr
    b. Sulfuric Acid (H_2SO_4): 70% concentration; the stoichiometry and required amount of sulfuric acid can be adjusted based on the reaction needs.

2. Reaction and Conversion:

    a. Reaction: $CH_3CH=CH_2 + H_2SO_4 \rightleftharpoons (CH_3)_2CHOSO_3H$
    b. Conversion: 70% of propylene reacts.
    c. Propylene Reacted: 0.7 * 34.967= 24.477 kmol/hr
    d. Unreacted Propylene: 34.967-24.477=10.49 Kmol/hr exits as part of the gas stream.

3. Products:

    a. Isopropyl Sulphate Formed: 24.477 Kmol/hr.
    b. Unreacted Components: 10.49 Kmol/hr of unreacted propylene.

<u>Material Balance Across the Hydrolyser and Stripper:</u>
In the hydrolyser, isopropyl sulphate reacts with water to form isopropanol (IPA) and regenerate sulfuric acid.

1. Feed to Hydrolyser:
   a. Isopropyl Sulphate: 24.477 Kmol/hr.
   b. Water (H_2O): Sufficient to convert the isopropyl sulphate completely to IPA.
2. Reaction:
   a. Reaction: $(CH_3)_2CHOSO_3H + H_2O \leftrightharpoons (CH_3)_2CHOH + H_2SO_4$
   b. Products:
      i. Isopropanol (IPA): 24.477 kmol/hr.
      ii. Regenerated Sulfuric Acid: Recycled back into the process.
3. Gas and Liquid Stream:
   a. IPA Vapors: 24.477 kmol/hr.
   b. Acidic Impurities: Small amounts, which are removed in the next stage.

Material Balance Across the Caustic Wash:
The purpose of the caustic wash is to remove acidic impurities from the IPA vapors.

1. Feed to Caustic Wash:
   a. IPA Vapors: 24.477 kmol/hr.
   b. Acidic Impurities: Minimal.
2. Output:
   a. Purified IPA Vapors: 24.477 kmol/hr, which are then sent to the condenser.

Material Balance Across the Condenser and Separation:
The condenser separates unreacted propylene from the IPA and ether mixture.

1. Feed to Condenser:
   a. Purified IPA Vapors: 24.477 kmol/hr.
   b. Unreacted Propylene: 10.49 kmol/hr.
2. Separation:
   a. Propylene Gas: 10.49 kmol/hr, which is recycled back to the absorber.
   b. IPA and Ether Mixture: Sent to the next separation step.

Material Balance Across the Ether Column:

In the ether column, isopropyl ether is separated from the isopropanol.

1. Feed to Ether Column:
   a. Isopropanol (IPA): 24.477 kmol/hr.
   b. Water (H_2O): A small amount may be present, but we'll assume this is negligible here.
2. Separation Products:
   a. Isopropyl Ether ($(CH_3)_2CHOCH(CH_3)_2$: Let's assume that 1% of IPA is converted to isopropyl ether during the separation.
   b. Remaining Isopropanol: 24.477 kmol/hr * 0.99 = 24.232 kmol/hr.
3. Output:
   a. Isopropyl Ether: 0.245 kmol/hr (recycled to the process).
   b. Isopropanol: 24.232 kmol/hr (goes to the IPA column).

Material Balance Across the IPA Column:

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

1. Feed to IPA Column:
   a. Isopropanol: 24.232 kmol/hr.
   b. Water Content: Assume it's negligible initially.
2. Separation Products:

    a. 87% Isopropanol (IPA) Mixture: 24.232 kmol/hr * 0.87 = 21.080 kmol/hr.

    b. Water Content: 24.232 kmol/hr * 0.13 = 3.152 kmol/hr.

3. Output:

    a. 87% IPA Mixture: 21.080 kmol/hr, goes to the azeotropic distillation column.

    b. Water and Waste: 3.152 kmol/hr, removed from the system.

Material Balance Across the Azeotropic Distillation Column:

In the azeotropic distillation column, 99% pure IPA is separated from water using isopropyl ether as an azeotropic agent.

1. Feed to Azeotropic Column:

    a. 87% IPA Mixture: 21.080 kmol/hr.

2. Separation Products:

    a. 99% Pure IPA: 20.869 kmol/hr (final product).

    b. Azeotropic Mixture of Ether and Water: 21.080 - 20.869 = 0.211 kmol/hr (recycled).

3. Output:

    a. 99% Pure IPA: 20.869 kmol/hr.

    b. Azeotropic Mixture (Ether and Water): 0.211 kmol/hr.

Summary of both method:

→ 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.

Now, we will Simulate the Direct Hydration Method:

SIMULATION OF DIRECT HYDRATION ON ASPEN:

a) A stoichiometric conversion reactor receives a feed of C_2H_6 and H_2O, both at 519 K, where the desired reaction takes place.

b) The product stream exiting the reactor at 523 K is passed through a heat exchanger to cool the gases down to 313 K.

c) In the next step, C_2H_6 is separated and recycled from the product stream, while the remaining mixture of IPA and water is sent to a distillation setup.

d) 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.

e) 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.

MATERIAL BALANCES THAT WE GOT ON ASPEN:

	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	54.8011
− Mole Flows	kmol/hr	**34.967**	**49.9529**	**99.9058**	**64.9388**	**64.9388**	**14.9859**	**49.9529**	**49**	**0.9529**	**45**	**4**	**40**
PROPY-01	kmol/hr	34.967	0	49.9529	14.9859	14.9859	14.9859	0	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	34.967
WATER	kmol/hr	0	49.9529	49.9529	14.9859	14.9859	0	14.9859	14.033	0.952898	10.033	3.99999	5.03304
BENZENE	kmol/hr	0	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	0
ISOPR-01		0	0	0	0.538461	0.538461	0	0.699999	0.713612	1.725e-06	0.777044	2.88536e-06	0.874174
WATER		0	1	0.5	0.23077	0.23077	0	0.300001	0.286388	0.999998	0.222956	0.999997	0.125826
BENZENE		0	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**	**2192.04**
PROPY-01	kg/hr	1471.43	0	2102.05	630.614	630.614	630.614	0	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	2101.37
WATER	kg/hr	0	899.915	899.915	269.975	269.975	0	269.975	252.808	17.1667	180.748	72.0609	90.6716
BENZENE	kg/hr	0	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	0
ISOPR-01		0	0	0	0.7	0.7	0	0.886151	0.892613	5.75429e-06	0.920798	9.62499e-06	0.958636
WATER		0	1	0.299776	0.0899329	0.0899329	0	0.113849	0.107387	0.999994	0.0792016	0.99999	0.0413639
BENZENE		0	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	50.55
+ Vapor Phase													

	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
Volume Flow	l/min	6499.83	49.8192	53.4767	0.311579	52.1688	1.30792	50.55	1.63491	1.67658	3.25441	4.93098	48.9198

ENERGY REQUIREMENTS OF DIRECT HYDRATION:
1)HEATER

Heater	Sep	RadFrac	RStoic	M

Henry's component list ID	
Electrolyte chemistry ID	
Use true species approach for electrolytes	YES
Free-water phase properties method	STEAM-TA
Water solubility method	3
Specified pressure [bar]	1
Specified temperature [K]	313
Specified vapor fraction	
Specified heat duty [cal/sec]	
EO Model components	
Calculated pressure [bar]	1
Calculated temperature [C]	39.85
Calculated vapor fraction	0.212616
Calculated heat duty [kJ/sec]	-815.041
Temperature change [C]	
Degrees of superheating [C]	
Degrees of subcooling [C]	
Pressure-drop correlation parameter	
Net duty [kJ/sec]	-815.041
First liquid / total liquid	1

2)SEPERATOR:

Heater	Sep	RadFrac	RStoic	M
Inlet flash pressure [bar]				0
First outlet flash temperature				
First outlet flash pressure				
First outlet flash temperature change				
First outlet flash vapor fraction				
First outlet flash temperature estimate				
First outlet flash pressure estimate				
Second outlet flash temperature				
Second outlet flash pressure				
Second outlet flash temperature change				
Second outlet flash vapor fraction				
Second outlet flash temperature estimate				
Second outlet flash pressure estimate				
EO Model components				
Heat duty [kJ/sec]		-9.45718		

3)DISTILLATION COLUMN:

| | Heater | Sep | **RadFrac** | RStoic | Mixer |

		▼	▼	▼	▼
Name	DISTCOL1	DISTCOL2	DISTCOL3	DISTCOL4
Property method	IDEAL	IDEAL	IDEAL	IDEAL
Henry's component list ID				
Electrolyte chemistry ID				
Use true species approach for electrolytes	YES	YES	YES	YES
Free-water phase properties method	STEAM-TA	STEAM-TA	STEAM-TA	STEAM-TA
Water solubility method	3	3	3	3
Number of stages	30	30	30	30
Condenser	TOTAL	TOTAL	TOTAL	TOTAL
Reboiler	KETTLE	KETTLE	KETTLE	KETTLE
Number of phases	2	2	2	2
Free-water	NO	NO	NO	NO
Top stage pressure [atm]	1	1	1	1
Specified reflux ratio	2.6	2.6	2.6	2.6
Specified bottoms rate [kmol/hr]				
Specified boilup rate [kmol/hr]				
Specified distillate rate [kmol/hr]	49	45	40	34.967
EO Model components				
Calculated molar reflux ratio	2.6	2.6	2.6	2.6
Calculated bottoms rate [kmol/hr]	0.9529	4	5	5.033
Calculated boilup rate [kmol/hr]	185.485	161.787	143.64	125.287
Calculated distillate rate [kmol/hr]	49	45	40	34.967

| Heater | Sep | **RadFrac** | RStoic | Mixer |

Calculated boilup rate [kmol/hr]	185.485	161.787	143.64	125.287
Calculated distillate rate [kmol/hr]	49	45	40	34.967
Condenser / top stage temperature [C]	85.9104	84.9936	83.6606	82.0584
Condenser / top stage pressure [bar]	1.01325	1.01325	1.01325	1.01325
Condenser / top stage heat duty [kJ/sec]	-1992.86	-1829.6	-1624.86	-1417.45
Condenser / top stage subcooled duty				
Condenser / top stage reflux rate [kmol/hr]	127.4	117	104	90.9142
Condenser / top stage free water reflux ratio				
Reboiler pressure [bar]	1.01325	1.01325	1.01325	1.01325
Reboiler temperature [C]	100.018	100.018	100.018	99.8648
Reboiler heat duty [kJ/sec]	2096.64	1828.77	1623.65	1416.02
Total feed stream CO2e flow [kg/hr]	0	0	0	0
Total product stream CO2e flow [kg/hr]	0	0	0	0
Net stream CO2e production [kg/hr]	0	0	0	0
Utility CO2e production [kg/hr]	0	0	0	0
Total CO2e production [kg/hr]	0	0	0	0

4)REACTOR:

	Heater	Sep	RadFrac	**RStoic**	Mixer

Electrolyte chemistry ID	
Use true species approach for electrolytes	YES
Free-water phase properties method	STEAM-TA
Water solubility method	3
Specified pressure [atm]	200
Specified temperature [K]	523
Specified vapor fraction	
Specified heat duty [cal/sec]	
EO Model components	
Outlet temperature [C]	249.85
Outlet pressure [bar]	202.65
Calculated heat duty [kJ/sec]	-545.821
Net heat duty [kJ/sec]	-545.821
Calculated vapor fraction	0
First liquid / total liquid	1
Total feed stream CO2e flow [kg/hr]	0
Total product stream CO2e flow [kg/hr]	0
Net stream CO2e production [kg/hr]	0
Utility CO2e production [kg/hr]	0
Total CO2e production [kg/hr]	0
Utility usage	
Utility cost	
Utility ID	

5)MIXER:

	Heater	Sep	RadFrac	RStoic	**Mixer**			
Name				B7		MIX1		MIX2
Property method				IDEAL		IDEAL		IDEAL
Henry's component list ID								
Electrolyte chemistry ID								
Use true species approach for electrolytes				YES		YES		YES
Free-water phase properties method				STEAM-TA		STEAM-TA		STEAM-TA
Water solubility method				3		3		3
Specified pressure [bar]					0		0	0
Temperature estimate [C]								
EO Model components								
Outlet temperature [C]					99.966		206.473	100.018
Calculated outlet pressure [bar]					1.01325		1	1.01325
Vapor fraction					0		1	0
First liquid /Total liquid					1		1	1
Total feed stream CO2e flow [kg/hr]					0		0	0
Total product stream CO2e flow [kg/hr]					0		0	0
Net stream CO2e production [kg/hr]					0		0	0

COST ANALYSIS

We tried to estimate the cost of such a plant if we planned to make one in near future

Raw materials =

We require 34.967 kmol/hr of propylene and water for our reaction so we calculate the price /hr of raw materials

Mass of propylene /hr= 1468.6 Kg

Mass of water /hr = 629.4 Kg

Price of propylene /hr = 3671535 INR

Price of water /hr = 17 INR

So total costing come around 36 Lakh INR/hr

Equipment costs

As seen in the flowchart we require **1 reactor 1 heat exchanger 1 separator 4 distilator 4 condensor 4 rebioler** in our process.

Cost of reactor to be around **1-1.5** Crores INR /per piece

Cost of Heat exchanger **12** Lakhs INR/per peice

Cost of seperator **10** Lakh./per piece

Cost of distillation **68** LAKH INR/per piece

Cost of condensor **10** Lakh INR/per piece

Cost of reboiler **15** LAKH INR/per piece

Total equipment costs = 2.5 Cr INR

We took it without all the electrical equipment and land and labour costings we estimated the running and operating cost to be ------

NET COST =SETup cost + Raw material cost

25000000+1450000000=
1475000000 INR/year

Production of IPA = 50000 Kg/ day
Round Year 365 days
Price of IPA =129 INR /Kg
Total income = 2354250000 INR/year

Gross income = 2354250000 −1475000000
=879250000

TAX of 30 @ Gross income =263775000

NET profit =879250000-263775000
=615475000