Technical Report

Company Name: ProChem Innovations

CEO: Nikhil Gupta

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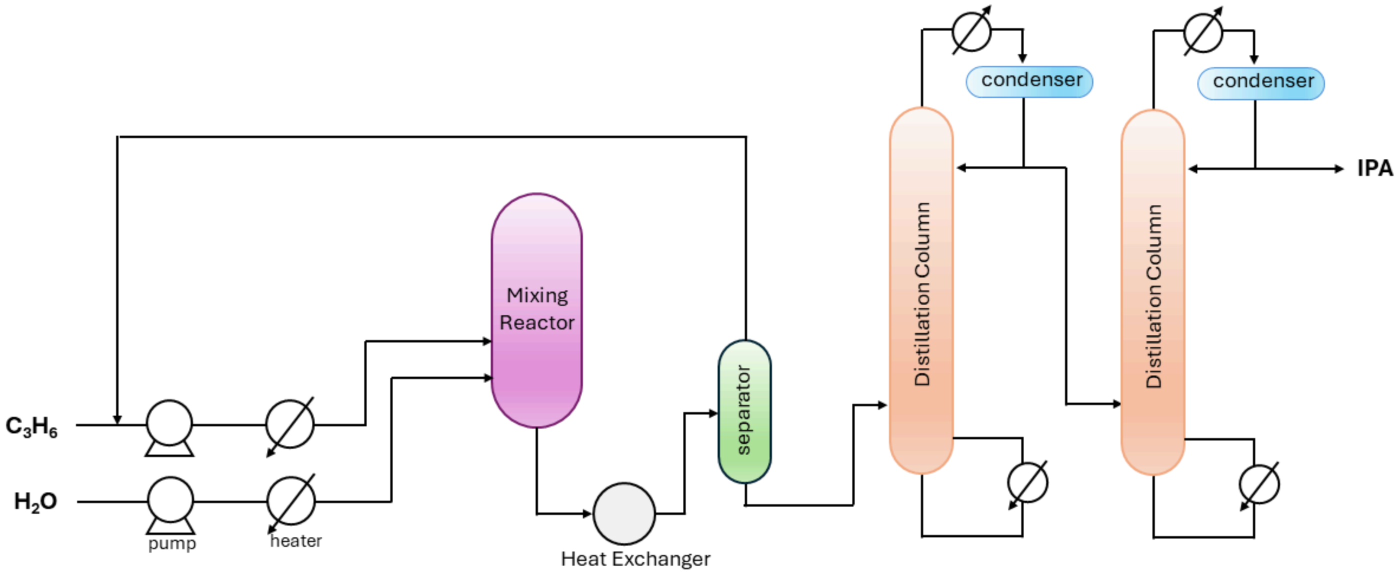
Chemical Formula: $(CH_3)_2CHOH$

Chemical Name: Isopropanol

Block Diagram:



1. Production Rate

1 ton of Isopropyl alcohol is produced every day.

41.67 kg of Isopropyl alcohol is produced every hour.

Therefore, 41.67 kg/hr of Isopropyl alcohol is produced.

2. Raw Material Requirement

From stoichiometry, to produce 41.67 kg/hr Isopropyl alcohol, i.e. 0.6945 kmol/hr we will require exactly the same amount of propylene and water (feed).

Therefore, 0.6945 kmol/hr of propylene and water is required as raw material.

Water is fed in 1:1 ratio to propylene

Amount of water required = 0.6945 x 1 = 0.6945 kmol/hr

Therefore, 0.6945 kmol/hr of air is required.

3. Material balance across individual equipments

3.1 Material balance across Reactor

Weight of $CH_3CH{=}CH_2$ entering= 0.6945 kmol/hr

Weight of H_2O entering= 0.6945 kmol/hr

Reaction occurring: $CH_3CH{=}CH_2 + H_2O \longrightarrow (CH_3)_2CHOH$

Amount of $CH_3CH{=}CH_2$ recycled = 0.20835 kmol/hr

Amount of $CH_3CH{=}CH_2$ entering the reactor= 0.90285 kmol/hr

Moles of H_2O entering= 0.6945 kmol/hr

Given single pass conversion for propylene in the reactor= 70%

Amount of $(CH_3)_2CHOH$ formed = 0.7*(0.90285) kmol of $CH_3CH{=}CH_2$

= 0.631995 kmol of $(CH_3)_2CHOH$

Amount of H_2O formed = 0.3*0.6945 kmol of H_2O

= 0.20835 kmol of H_2O

Compounds	Material entering (kmol/h)	Inside reactor (kmol/h)	Material leaving (kmol/h)
Propylene	0. 9921	-0.6945	0.2976
Water	0. 9921	-0.6945	0.2976
Isopropyl alcohol	0	0.6945	0.6945
Total	1.9842	-0.6945	1.2897

3.2 Material Balance across Heat Exchanger

Compounds	Material entering (kmol/h)	Material leaving (kmol/h)
Propylene	0.2976	0.2976
Water	0.2976	0.2976
Isopropyl Alcohol	0.6945	0.6945
Total	1.2897	1.2897

3.3 Material Balance across Separator

Amount of C_3H_6 entering= 0.2976 kmol/hr

Amount ofC_3H_6 Recycled= 0.2976 kmol/hr

Amount of C_3H_6 leaving = 0 kmo/hr

Compounds	**Material entering (kmol/h)**	**Recycle (kmol/h)**	**Material leaving (kmol/h)**
Propylene	0.2976	0.2976	0
Water	0.2976	0	0.2976
Isopropyl Alcohol	0.6945	0	0.6945
Total	1.2897	0.2976	0.9921

3.4 Material balance across Distillation Column

We need 99% pure Isopropyl alcohol (literature) i.e 1% water comes out with Isopropyl alcohol.

Amount of H2O entering = 0.20835 kmol/hr

Amount of C3H8O entering = 0.6945 kmol/hr

Moles of H2O leaving (top) = 0.01*0.6945 = 0.006945 kmol/hr

Amount of C3H8O Leaving (top) having 99% purity = 0.6945 kmol/hr

Amount of H2O leaving the bottom stream= 0.201405 kmol/hr

Compounds	**Material entering (kmol/h)**	**Top stream (kmol/h)**	**Bottom stream (kmol/h)**
Propylene	0	0	0
Water	0.2976	0.006945	0.290655
Isopropyl Alcohol	0.6945	0.687555	0.006945
Total	0.9921	0.6945	0.304545

4. Overall Material Balance

Compounds	**Material entering (kmol/h)**	**Material leaving (kmol/h)**
Propylene	0.6945	0
Water	0.9921	0.2976
Isopropyl Alcohol	0	0.6945
Total	1.6866	0.9921

5. Energy balance across individual equipments

5.1 Energy balance across Reactor

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

P1= 1 atm

P2= 200 atm

R= 0.0821 L.atm/K.mol

Cp= 84.5495

T2= 250° C

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

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

T1= 246° C

	ENTERING					**LEAVING**			
	Mass flow rate kmol/hr)	**Specific Heat kJ/kmol-**	**T (K)**	**Energy (kJ/s)**		**Mass flow rate kmol/hr)**	**ecific at (kJ/kmol-**	**T (K)**	**Energy (kJ/s)**
C3H6	0.9921	31.0667	519	8.8855		0.2976	131.733	523	2.7225
H_2O	0.9921	90.666	519	6.1466		0.2976	90.666	523	1.8738
IPA	-	-	-	-		0.6945	375.4043	523	18.1054
	TOTAL			15.0321		**TOTAL**			22.7017

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=7.6696 kJ/s

	TOTAL ENERGY ENTERING (kJ/s)	**TOTAL ENERGY LEAVING (kJ/s)**
Reactants enthalpies	15.0321	-
Products enthalpies	-	22.7017
Heat of reaction	7.6696	-
Heat transferred	-	-
TOTAL	22.7017	22.7017

5.2 Energy balance across Heat Exchanger

	ENTERING					**LEAVING**			
	Mass flow rate (kmol/hr)	**Specific Heat (kJ/kmol-**	**T (K)**	**Energy (kJ/s)**		**Mass flow rate (kmol/hr)**	**Specific Heat (kJ/kmol-**	**T (K)**	**Energy (kJ/s)**
C_3H_6	0.2976	131.733	523	2.7225		0.2976	103.733	313	0.3430
H_2O	0.2976	90.666	523	1.8738		0.20835	74.43	313	0.1723
IPA	0.6945	375.4043	523	18.1054		0.6945	169.5153	313	1.3081
	TOTAL			22.7017		**TOTAL**			1.8234

From energy balance equation,

Total Energy Leaving= Total Energy Entering

Energy Out = Energy In + Heat of Reaction + Q

1.8234=22.7017+0+Q

Q = -20.8783 kJ/s

Heat transferred out of the product mixture to cool the gases to a temperature of 40^{0} C and subsequently generate liquid is 20.8783 kJ/s

Water at a temperature of 283 K is required to cool the gases.

Heat transferred out of the gases = Sensible and latent heat gained by water

20.8783 = [mCp1 (T2-T1) + m λ + mCp2 (T3-T2)]

20.8783 = m*[75.766*(273-283) + 40680+ 76.32x(383-273)] m = 0.0004321 kmol/s

m = 1.55558 kmol/h

Mass of chilled water (coolant) required to cool down the gases is 1.55558 kmol/h

	TOTAL ENERGY ENTERING (kJ/s)	**TOTAL ENERGY LEAVING (kJ/s)**
Inlet energy	22.7017	-
Outlet energy	-	1.8234
Heat of reaction	-	-
Heat transferred	-	20.8783 (cooling)
TOTAL	22.7017	22.7017

5.3 Energy balance across 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)**
H_2O	0.006945	75.6576	363	0.0131		0.006945	75.2661	323	0.0073
IPA	0.6945	218.5365	363	3.7943		0.6945	165.0554	323	1.5921
	TOTAL			3.8074		**TOTAL**			1.5994

From energy balance equation,

Total Energy Leaving= Total Energy Entering

Energy Out = Energy In + Heat of Reaction + Q

1.5994 = 3.8074 + 0 + Q

Q = -2.208 kJ/s

Heat transferred out of the product mixture to cool the vapours to a temperature of 30^0 C and subsequently generate liquid is 2.208 kJ/s

Water at a temperature of 283 K is required to cool the vapours.

Heat transferred out of the gases= Sensible and latent heat gained by water

2.208 = mCp1 (T2-T1)

2.208 = m*[75.366*(333-283)]

m =0.00058594 kmol/s

m = 2.109384 kmol/h

Mass of chilled water (coolant)required to cool down the gases is 2.109384 kmol/h

	TOTAL ENERGY ENTERING (kJ/s)	**TOTAL ENERGY LEAVING (kJ/s)**
Inlet energy	3.8074	-
Outlet energy	-	1.5994
Heat of reaction	-	-
Heat transferred	-	2.208 (Condensation)
TOTAL	3.8074	3.8074

5.4 Energy balance across Reboiler

	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)**
H_2O	0.201405	75.312	333	0.2528		0.201405	75.7224	378	0.4448
	TOTAL			0.2528		**TOTAL**			0.4448

From energy balance equation,

Total Energy Leaving= Total Energy Entering

Energy Out = Energy In + Heat of Reaction + Q

0.4448 = 0.2528 + 0 + Q

Q = 0.192 kJ/s

Reboiler duty = 0.192 kW

	TOTAL ENERGY ENTERING (kJ/s)	TOTAL ENERGY LEAVING (kJ/s)
Inlet energy	0.2528	-
Outlet energy	-	0.4448
Heat of reaction	-	-
Heat transferred	0.192	-
TOTAL	0.2528	0.2528

6. Equipment costs

S.No.	Equipment	Quantity	Cost (in INR)
1	Pump	2	817,810
2	Reactor	1	12,258,805
3	Heater	2	114,610,230
4	Heat Exchanger	2	3,605,040
5	Separator	1	1,326,855
4	Distillation Column	2	30,714,285
5	Condenser	2	1,430,742
6	Reboiler	2	5,460,714
	TOTAL		**170,224,481**

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Contribution of each author:

- Author 1 developed the block diagram for the scaled up process and evaluated the approximate capital cost.
- Author 2 performed material and energy balance and identified the unit operations and operating conditions.

Signature:

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Technical Report

Company Name: ProChem Innovations

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Report Authors: 1. Pranshu Kumar (220799)

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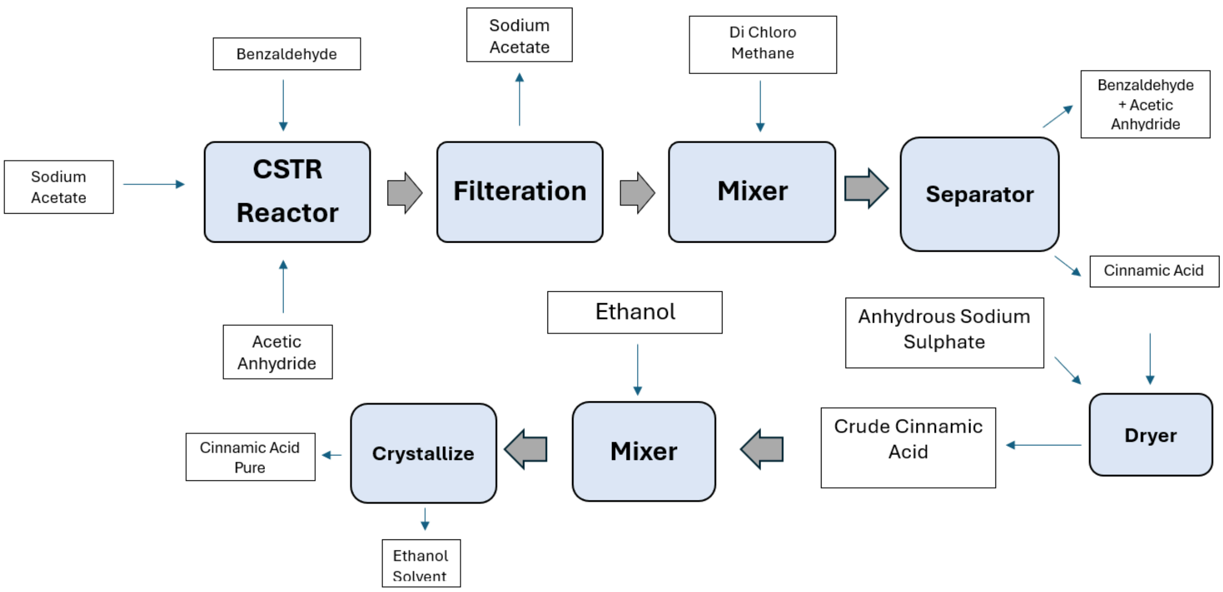
Chemical Formula: $C_9H_8O_2$

Chemical Name: Cinnamic Acid

Block Diagram:



1. Production Rate

1000 kg of Cinnamic Acid is produced everyday.

Therefore, the production rate of Cinnamic Acid is 41.67 kg/hr.

2. Raw Material Requirement

Ideally, from stoichiometry, to produce 41.67 kg/hr Cinnamic Acid, i.e. 0.2813 Kmol/hr we will require exactly the same amount of benzaldehyde and acetic anhydride (feed). But, the product conversion is not observed to be 100%.

Typically, the product conversion for the reaction is observed to be around 70%.

Amount of benzaldehyde required = 0.2813/(0.7) Kmol/hr = 0.4018 Kmol/hr

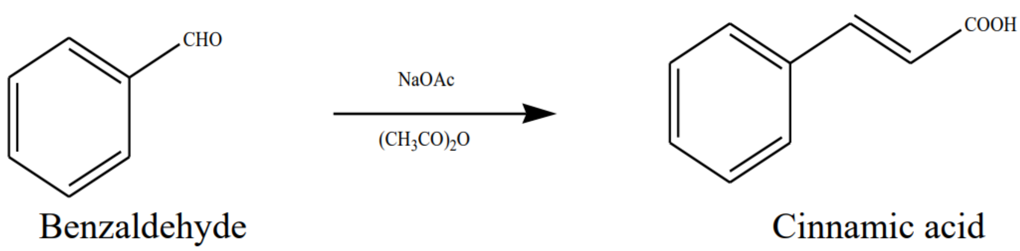
Therefore, the required flow rate for benzaldehyde and acetic anhydride will be 0.4018 Kmol/hr.

The amount of sodium acetate is typically around 3%mol, i.e., we would require the flow rate of sodium acetate to be 12.054 mol/hr.

3. Material balance across individual equipments

3.1. Material balance across Reactor

Reaction:



Amount of benzaldehyde entering= 0.4018 kmol/hr

Amount of acetic anhydride entering= 0.4018 kmol/hr

Component	**Material Entering (Kmol/h)**	**Material Leaving (Kmol/h)**
Benzaldehyde	0.4018	0.1205
Acetic Anhydride	0.4018	0.1205
Cinnamic Acid	0	0.2813
Sodium Acetate	0.0120	0.0120
Total	0.8156	0.5343

3.2. Material Balance across Filter

Component	Material Entering (Kmol/h)	Material Leaving (Kmol/h)	Stream Leaving (Kmol/h)
Benzaldehyde	0.1205	0.1205	0
Acetic Anhydride	0.1205	0.1205	0
Cinnamic Acid	0.2813	0.2813	0
Sodium Acetate	0.0120	0	0.0120
Total	0.5343	0.5123	0.0120

The sodium acetate can be reused as the catalyst in the reaction. Generally, sodium acetate can be used 3-4 times without losing its activity.

3.3. Material Balance across Mixer

Component	Material Entering (Kmol/h)	Stream Entering (Kmol/h)	Material Leaving (Kmol/h)
Benzaldehyde	0.1205	0	0.1205
Acetic Anhydride	0.1205	0	0.1205
Cinnamic Acid	0.2813	0	0.2813
Sodium Acetate	0	0	0
Dichloromethane	0	0.5000	0.5000
Total	0.5123	0.5000	1.0123

3.4. Material Balance across Separator

Component	Material Entering (Kmol/h)	Stream Leaving (Kmol/h)	Material Leaving (Kmol/h)

Benzaldehyde	0.1205	0.1205	0
Acetic Anhydride	0.1205	0.1205	0
Cinnamic Acid	0.2813	0	0.2813
Dichloromethane	0	0	0.5000
Total	0.5123	0.2410	0.7813

3.5. Material Balance across Dryer

In the dryer, anhydrous sodium sulphate is added in small amounts as the drying agent.

Component	Material Entering (Kmol/h)	Material Leaving (Kmol/h)
Cinnamic Acid	0.2813	0.2813
Dichloromethane	0.5000	0
Total	0.7813	0.2813

3.6. Material Balance across Mixer

Component	Material Entering (Kmol/h)	Stream Entering (in Kmol/h)	Material Leaving (Kmol/h)
Cinnamic Acid	0.2813	0	0.2813
Ethanol	0	0.5000	0.5000
Total	0.2813	0.5000	0.7813

3.7. Material Balance across Crystallizer

Component	Material Entering (Kmol/h)	Stream Leaving (in Kmol/h)	Material Leaving (Kmol/h)
Cinnamic Acid	0.2813	0	0.2813
Ethanol	0.5000	0.5000	0
Total	0.2813	0.5000	0.2813

The final product obtained from the crystallizer has high purity.

4. Overall Material Balance

Component	Material Entering (Kmol/h)	Material Leaving (Kmol/h)
Benzaldehyde	0.4018	0.1205
Acetic Anhydride	0.4018	0.1205
Cinnamic Acid	0	0.2813
Total	0.8036	0.5223

The Benzaldehyde and Acetic Anhydride obtained can be reused as the reactants to produce Cinnamic Acid.

5. Equipment costs

S.No.	Equipment	Quantity	Cost (in INR)
1	Separator	1	1,326,855
2	Distillation Column	1	15,357,142
3	Crystallize	1	3,730,396
4	Mixer	2	4,022,484
5	Dryer	1	5,399,477

6	Filter	1	33,231,402
	TOTAL		**63,067,756/-**

6. Material Cost:

S.No.	Material	Rate(per kg)	Quantity (per h)	Cost (in INR)
1	Sodium Acetate	20	0.9842	19.684
2	Benzaldehyde	140	42.6390	5969.46
3	Acetic anhydride	50	41.0197	2050.985
4	Ethanol	65	23.03	1496.9500
5	Di-Chloro Methane	85	42.465	3609.5250
	Total			13146.604

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[3]https://pubchem.ncbi.nlm.nih.gov/compound/Cinnamic-Acid%26amp;sa%3DD%26amp;source%3Deditors%26amp;ust%3D1712217543647679%26amp;usg%3DAOvVaw1qfsYRxzq7aORwi6lAsT81&sa=D&source=docs&ust=1712217543671827&usg=AOvVaw2Gmbflii9AxTGDiBEzMFmm

[4]http://www.matche.com/equipcost/Default.html

Contribution of each author:

- Author 1 developed the block diagram for the scaled up process and evaluated the approximate capital cost.
- Author 2 performed material and identified the unit operations and operating conditions.

Signature:

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