

Efficient and Cost-effective Production of Isopropyl Alcohol using Tokuyama Soda Process: Design and Analysis of a Chemical Engineering Plant

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Abstract: In this study, a chemical engineering plant for the production of Isopropyl Alcohol (IPA) using the Tokuyama Soda Process has been designed. The feasibility of the process was analyzed using thermodynamic principles, and a detailed heat and mass balance were performed to determine the optimal conditions for the production of IPA. The design of key equipment such as the distillation column, heat exchanger, condenser, and reactor were also carried out. A Process and Instrumentation Diagram (PID) was developed to illustrate the process flow and control systems. Finally, a cost analysis was conducted to estimate the capital and operating costs of the plant. The results of the study show that the designed plant has the potential to produce IPA efficiently and cost-effectively, meeting the quality requirements of the target market. The study demonstrates the importance of thorough analysis and design in developing efficient and effective chemical engineering processes.

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Isopropyl alcohol was first produced by Standard oil in 1920 by hydrating propene. Its major use at the time was not rubbing alcohol but for oxidation to acetone, whose first major use was in World War I for the preparation of cordite, a smokeless, low explosive propellant. The discovery of isopropyl alcohol happened quite early though it wasn't very significant at that time. IPA's distillation process was discovered in the first century and it was available for consumption and uses in the medical field as well. The first industrial process happened in 1926, which was the base for different alcohols through chemical synthesis. Scrolls have been found that were made by the Ancient Egyptians that gives directions to produce beer from plant foods and IPA was commonly found in the drink however it was referred to as ethanol.

1.1 About the compound

Isopropyl alcohol, also called **2-propanol**, one of the most common members of the alcohol family of organic compounds is manufactured from propylene as shown in Figure 1.1. Isopropyl alcohol was the first commercial synthetic alcohol. Isopropyl alcohol (IUPAC name propan-2-ol) is a colorless, flammable chemical compound (chemical formula $\text{CH}_3\text{CHOHCH}_3$) with a strong odor. As an isopropyl group linked to a hydroxyl group, it is the simplest example of a secondary alcohol, where the alcohol carbon atom is attached to two other carbon atoms. It is a structural isomer of 1-propanol and ethyl methyl ether.

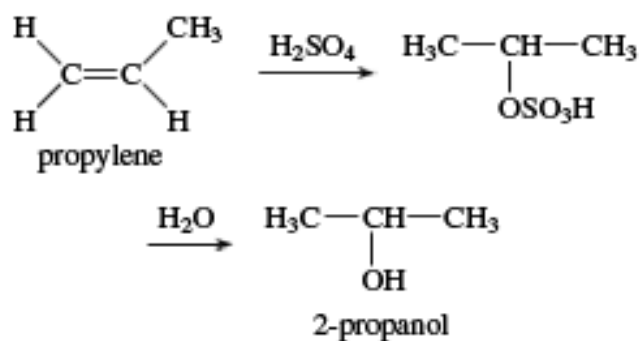


Figure 1.1 Isopropyl alcohol from propylene ^[1]

Isopropyl alcohol is miscible in water, ethanol, ether, and chloroform. It dissolves ethyl cellulose, polyvinyl butyral, many oils, alkaloids, gums and natural resins. Unlike ethanol or methanol, isopropyl alcohol is not miscible with salt solutions and can be separated from aqueous solutions by adding a salt such as sodium chloride. The process is

colloquially called salting out, and causes concentrated isopropyl alcohol to separate into a distinct layer.

It is used in the manufacture of a wide variety of industrial and household chemicals, and is a common ingredient in chemicals such as antiseptics, disinfectants, and detergents.

1.2 Growth and demand

1.2.1 Market analysis of the compound

The global isopropyl alcohol market reached a value of US\$ 3.8 Billion in 2018, registering a CAGR of 5.7% during 2011-2018. The market value is further anticipated to reach US\$ 4.8 Billion by 2024, exhibiting a CAGR of nearly 4% during 2019-2024. On the basis of the industry, the market has been divided into cosmetic and personal care, pharmaceutical, food and beverage, paints and coatings, chemical, and others. Amongst these, isopropyl alcohol finds extensive application in the chemical industry as an intermediate and cleaning agent.

- Region-wise, Asia represents the largest market for isopropyl alcohol around the world. This can be accredited to the burgeoning personal care and cosmetics industry in the region. Isopropyl alcohol is used in the production of skin cleansers and lotions, deodorants, nail paints, hair tonics and shampoos. Other major markets include North America, Europe and South America.
- On assessing the import and export scenario of the market, it has been found that the United States represents the biggest importer and exporter of isopropyl alcohol.
- The competitive landscape of the market has been examined with some of the key players being The Dow Chemical Company, Exxon Mobil Corporation, Shell Chemicals Europe B.V., INEOS Enterprises Group Limited and Super Chemical Technology Co. Ltd.
- Figure 1.2 shows the annual production of Isopropyl Alcohol from 1990-2018

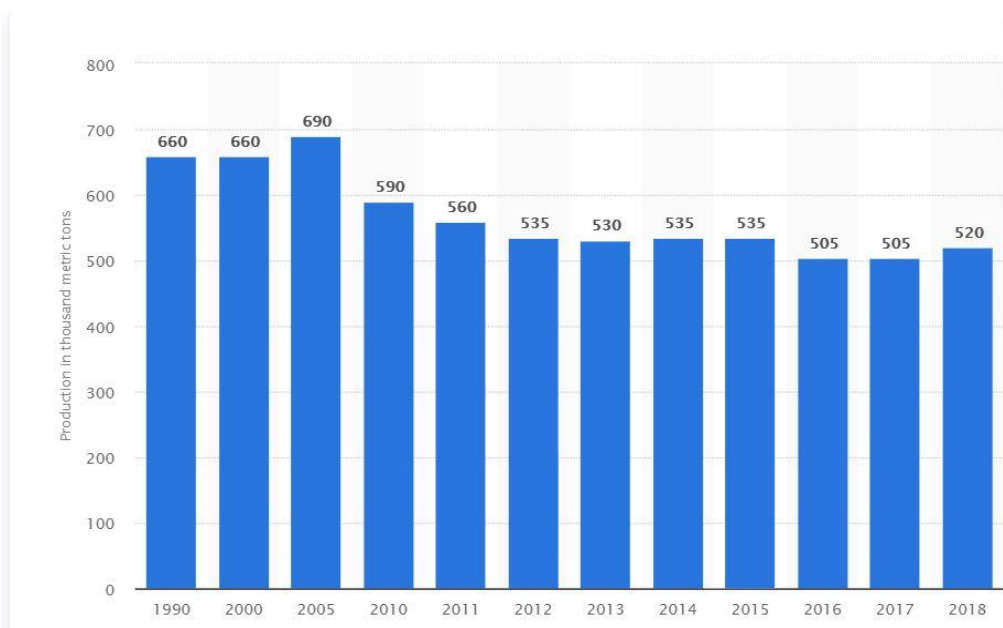


Figure 1.2 Annual production of Isopropyl Alcohol (1990-2018) [2]

1.2.2 Immense growth potential in India

In India, pharmaceutical industry, the largest driver for iso-propanol, shows promising growth and expected to be the primary factor in the rise of iso-propanol growth. Chemical industry, and coating and ink industry are other major end consumers of iso-propanol in the country, which are also expected to grow in the coming years. Southern and eastern regions are also expected to drive the demand for iso-propanol in the coming years due to a rise in the pharmaceutical industry in these regions.

Demand for iso-propanol has recorded impressive growth rates. The only domestic producer of IPA is, Deepak Fertilizers and Petrochemicals Corporation Limited, which has an installed capacity of 70,000 metric tons per annum and commenced production from 2006. Globally, the demand growth of Isopropanol is majorly driven by its use in cosmetics, household products and pharmaceutical industries. North America leads production as well as consumption of Isopropanol while Asia-Pacific is the largest consumer. India and China are among the top growing markets of Isopropanol for the pharmaceutical applications as shown in figure 1.3.

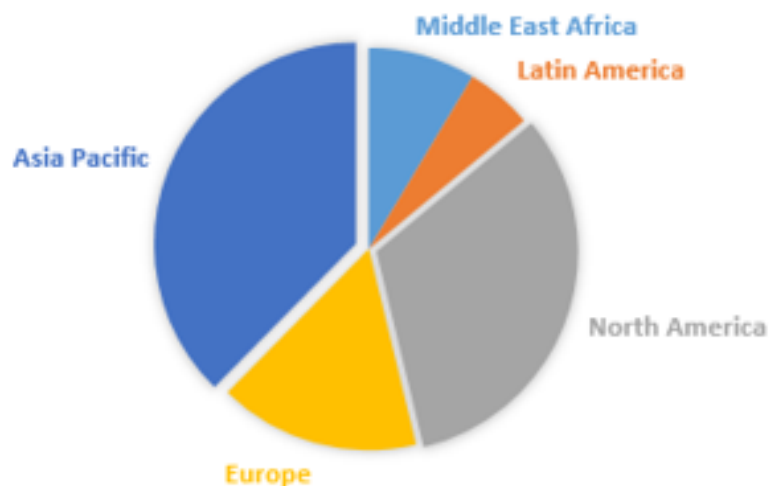


Figure 1.3 Isopropyl alcohol market by region ^[3]

1.3 Applications

- *Solvent*: Isopropyl alcohol dissolves a wide range of non polar compounds. It also evaporates quickly, leaves nearly zero oil traces, compared to ethanol, and is relatively non-toxic, compared to alternative solvents.
- *Intermediate*: Isopropyl alcohol is esterified to give isopropyl acetate, another solvent. It reacts with carbon di sulfide and sodium hydroxide to give sodium isopropylxanthate, a herbicide and an ore flotation reagent.
- *Medical*: Rubbing alcohol, hand sanitizer, and disinfecting pads typically contain a 60–70% solution of isopropyl alcohol or ethonal in water. Isopropyl alcohol is used as a water-drying aid for the prevention of otitis externa, it can also be used as an anesthetic.
- *Automotive*: Isopropyl alcohol is a major ingredient in "gas dryer" fuel additives. In significant quantities water is a problem in fuel tanks, as it separates from gasoline and can freeze in the supply lines at low temperatures.
- *Laboratory*: As a biological specimen preservative, isopropyl alcohol provides a comparatively non-toxic alternative to formaldehyde and other synthetic preservatives. Isopropyl alcohol solutions of 70–99% are used to preserve specimens.

Isopropyl alcohol is often used in DNA extraction. A lab worker adds it to a DNA solution to precipitate the DNA, which then forms a pellet after centrifugation. This is possible because DNA is insoluble in isopropyl alcohol.

1.4 Toxic effects of the compound

- Clinical effects:
 - Drowsiness, ataxia and stupor.
 - Coma and respiratory depression.
 - Irritation of mucous membranes and eyes.
- High risk circumstances of poisoning:
 - Accidental ingestion of rubbing alcohols/toiletries by children.
 - Occupational or accidental exposure to liquid or its vapour.
- Routes of exposure:
 - Oral ingestion of rubbing alcohols and toilet preparations, constitute the most common route of exposure. Doses of above 20 mL may produce toxic effects.
 - Dermal exposure to the liquid and vapour. There is little absorption through intact skin, but significant delayed absorption over 4 hours postulated.
 - Eye exposure to liquid and vapour. Both the liquid and solvent are severely irritant.
- Mode of action:
 - Isopropyl alcohol is an irritant to mucous membranes and eyes.
 - Isopropyl alcohol is a potent central nervous system (CNS) depressant, and in large doses causes cardiovascular depression.
 - Inebriation, peripheral vasodilation and hypothermia may also occur.

1.5 Objective and scope

The present project on production of 50 tons/day of Isopropyl alcohol by hydration of propylene will be based on following objectives.

- To execute a detailed literature survey of various processes used in the manufacture of Isopropyl alcohol.
- To carry out thermodynamic feasibility studies for the selected process.
- To study the material balance for the process.
- To study the energy balance for the process.

- To do the process and mechanical design of equipments used in the process.
- To study the cost estimation and economics.
- To prepare the plant location and layout report.
- To prepare the PID, pollution and safety details for the process.

A detailed study about Isopropyl Alcohol and its various production methods was studied by analyzing individual sources. In this chapter we have identified the best process used for the production of Isopropyl alcohol.

2.1 About the compound

Isopropyl alcohol, also called **2-propanol**, one of the most common members of the alcohol family of organic compounds. Isopropyl alcohol was the first commercial synthetic alcohol.

Isopropyl alcohol is miscible in water, ethanol, ether, and chloroform. It dissolves ethyl cellulose, polyvinyl butyral, many oils, alkaloids, gums and natural resins. Unlike ethanol or methanol, isopropyl alcohol is not miscible with salt solutions and can be separated from aqueous solutions by adding a salt such as sodium chloride. The process is colloquially called salting out, and causes concentrated isopropyl alcohol to separate into a distinct layer.

It is used in the manufacture of a wide variety of industrial and household chemicals, and is a common ingredient in chemicals such as antiseptics, disinfectants, and detergents.

Isopropyl alcohol (IUPAC name propan-2-ol; commonly called isopropanol or 2-propanol) is a colorless, flammable chemical compound (chemical formula $\text{CH}_3\text{CHOHCH}_3$) with a strong odor. As an isopropyl group linked to a hydroxyl group, it is the simplest example of a secondary alcohol, where the alcohol carbon atom is attached to two other carbon atoms as shown in Figure 2.1. It is a structural isomer of 1-propanol and ethyl methyl ether.

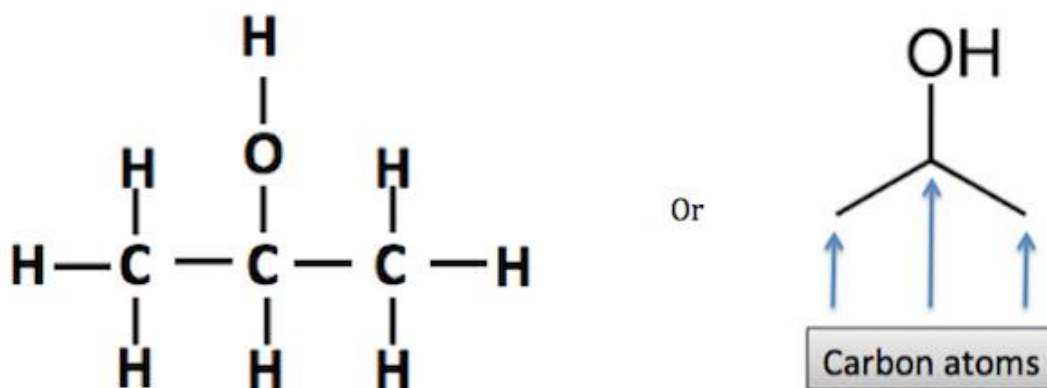


Figure. 2.1 Structure of Isopropyl alcohol [4]

2.2 Physical properties

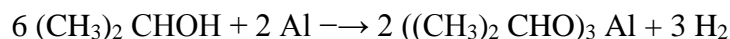
Figure 2.2 gives us the physical properties of isopropyl alcohol

Property	Anhydrous	91 Vol %
molecular weight	60.10	
boiling point, at 101.3 kPa ^b , °C	82.3	80.4
freezing point, °C	-88.5	-50.0
specific gravity, 20/20	0.7864	0.8183
density, at 20°C, g/cm ³	0.7854	0.8173
surface tension, at 20°C, mN/m(= dyn/cm)	21.32	21.40 ^c
specific heat, liquid at 20°C, J/(kg.K) ^d	2510.4	
refractive index, n ²⁰ _D	1.3772	1.3769
heat of combustion, at 25°C, kJ/mol ^d	2005.8	
latent heat of vaporization, at 101.3 kPa ^b , kJ/mol ^d	39.8	
vapor pressure, at 20°C, kPa ^b	4.4	4.5
critical temperature, °C	235.2	
critical pressure, at 20°C, kPa ^b	4764	
viscosity, mPa·s(= cP)		
at 0°C	4.6	
20°C	2.4	2.1 ^c
40°C	1.4	
coefficient of expansion ^e	$V_t = V_0[1 + (1.0743 \times 10^{-3})t + (3.28 \times 10^{-7})t^2]$	
flammability limit in air, vol % ^f		
lower	2.5	
upper	12	
flash point, °C		
Tag open cup	17.2	21.7
closed cup	11.7	18.3
autoignition temperature, °C ^g	399	

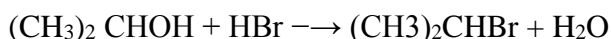
Fig 2.2 Physical properties of isopropyl alcohol ^[1]

2.3 Chemical properties

Chemical properties of isopropyl alcohol are determined by its functional hydroxyl group in the secondary position. Except for the production of acetone, most isopropyl alcohol chemistry involves the introduction of the isopropyl or isopropoxy group into other organic molecules by the breaking of the C–OH or the O–H bond in the isopropyl alcohol molecule. Isopropyl alcohol undergoes reactions typical of an active secondary alcohol. It can be dehydrogenated, oxidized, esterified, etherified, aminated, halogenated, or otherwise modified at the OH moiety more readily than primary alcohols such as n-propyl or ethyl alcohol. Manufacture of the commercially important aluminum isopropoxide and isopropyl halides illustrates this reactivity. The aluminum isopropoxide reaction involves the aluminum replacement of the hydroxyl hydrogen atom and concomitant hydrogen evolution; the isopropyl halides reaction involves hydroxyl group displacement. Aluminum isopropoxide is produced in quantitative yield by refluxing isopropyl alcohol with aluminum turnings.



Catalytic amounts of mercuric chloride are usually employed in this preparation. Aluminum isopropoxide is a useful Meerwein-Ponndorf-Verley reducing agent in certain ester-exchange reactions and is a precursor for aluminum glycinate, a buffering agent. Displacement of the hydroxyl group is exemplified by the production of isopropyl halides, eg, isopropyl bromide, by refluxing isopropyl alcohol with a halogen acid, eg, hydrobromic acid.



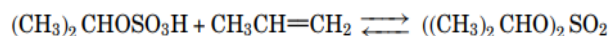
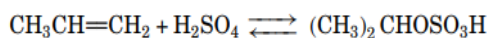
The order of reactivity with acid is $\text{HI} > \text{HBr} > \text{HCl}$. Reaction with hydrochloric acid to form isopropyl chloride is facilitated by a zinc chloride catalyst.

2.4 Different processes for the manufacture of Isopropyl alcohol

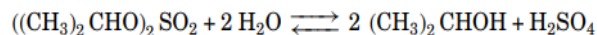
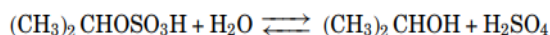
2.4.1 Indirect Hydration

This process is based on a two-step reaction of propylene and sulfuric acid. In the first step, mixed sulfate esters, primarily isopropyl hydrogen sulfate, but also diisopropyl sulfate, form. These are then hydrolyzed, forming the alcohol and sulfuric acid.

Step 1. Esterification:



Step 2. Hydrolysis:



In the process, propylene reacts with sulfuric acid (>60 wt%) in agitated reactors or absorbers at moderate (0.7–2.8 MPa (100–400 psig)) pressure. The isopropyl sulfate esters form and are maintained in the liquid state at 20–80°C. Because the reaction is exothermic, internal cooling coils or external heat exchangers are used to control the temperature. There are two general operational

modes for conducting the reaction. In the two-step strong acid process, separate reactors are used for the propylene absorption and sulfate ester hydrolysis stages. The reaction occurs at high sulfuric acid concentration (>80 wt%), at 1–1.2 MPa (130–160 psig) pressure, and low (eg, 20–30°C) temperature. The weak acid process is conducted in a single stage at low acid (60–80 wt %) concentration and at higher (2.5 MPa (350 psig)) pressure and (60–65°C) temperature. The sulfate ester hydrolysate is stripped to give a mixture of isopropyl alcohol, isopropyl ether, and water overhead, and dilute sulfuric acid bottoms. The overhead is neutralized using sodium hydroxide and refined in a two-column distillation system. Diisopropyl ether is taken overhead in the first, ie, ether, column.

This stream is generally recycled to the reactors to produce additional isopropyl alcohol by the following equilibrium reaction:



Wet isopropyl alcohol (87 wt % and 91 vol %) is taken overhead in the second still.

93% of the charged propylene is converted to isopropyl alcohol in this system.

The bottoms from the stripper (40–60 wt % acid) are sent to an acid reconcentration unit for upgrading to the proper acid strength and recycling to the reactor. Because of the associated high energy requirements, reconcentration of the diluted sulfuric acid is a costly operation.

Acid corrosion presents a problem in isopropyl alcohol factories. Steel (qv) is a satisfactory material of construction for tanks, lines, and columns where concentrated (>65 wt%) acid and moderate. Figure 2.3 shows the flowchart for the indirect hydration process for the manufacture of Isopropyl alcohol.

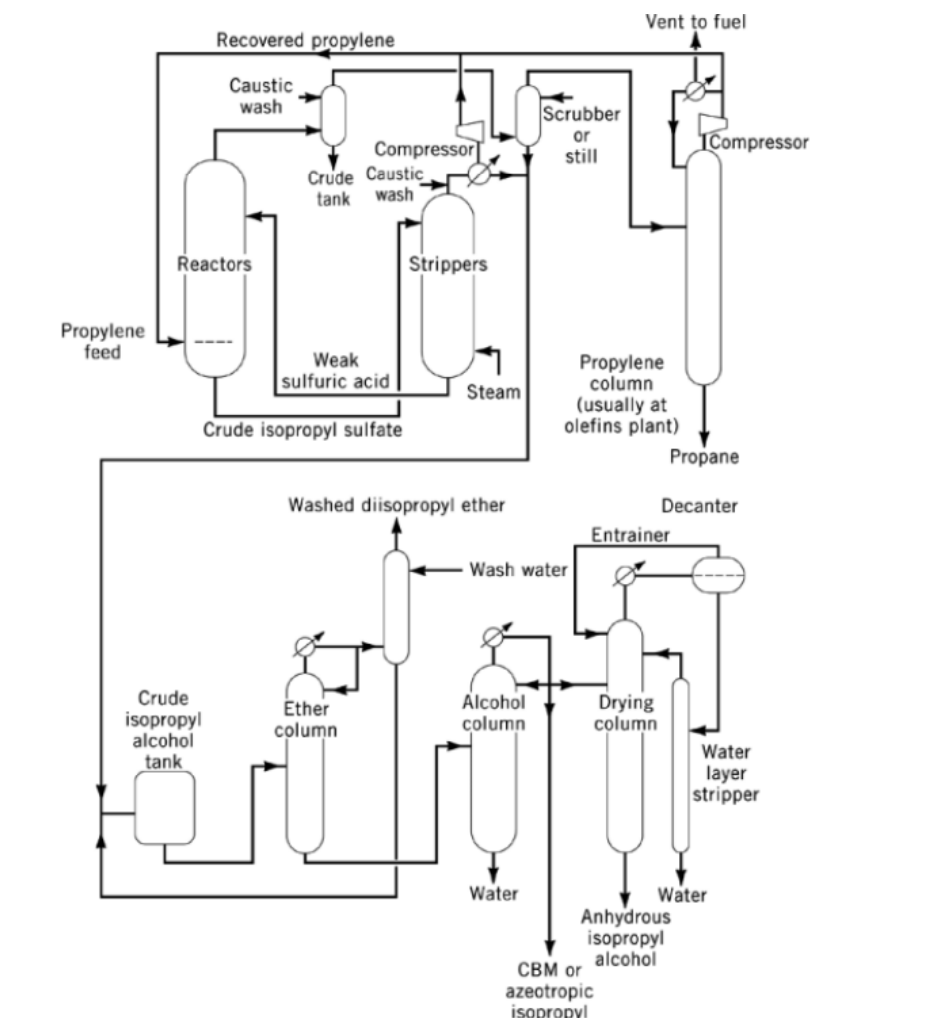
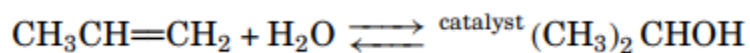


Figure 2.3

Indirect hydration process for the manufacture of isopropyl alcohol ^[1]

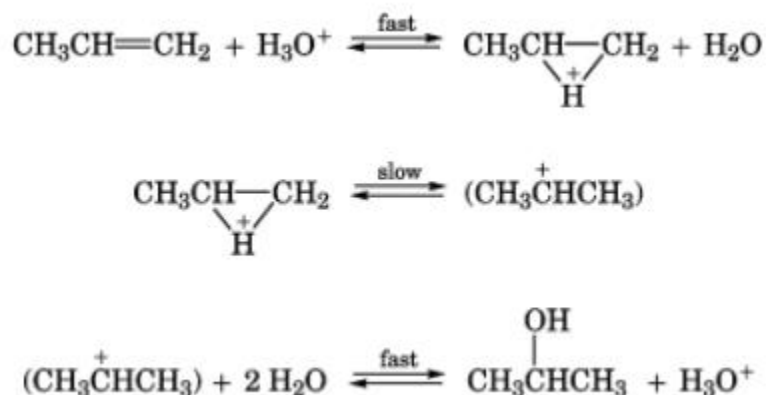
2.4.2 Direct Hydration

The acid-catalyzed direct hydration of propylene is exothermic and resembles the preparation of ethyl alcohol from ethylene.



The equilibrium can be controlled to favor product alcohol if high pressures and low temperatures are applied. The advantage of low temperature is difficult to utilize, however, because most known catalysts require high or moderate temperatures to be effective.

Propylene hydration in dilute acid solution probably proceeds according to the rate-determining formation of propyl carbonium ion. According to this mechanism, the reaction rate is proportional to the concentration of hydronium ion and is independent of the associated anion, ie, $\text{rate} = k[\text{CH}_3\text{H}_6][\text{H}_3\text{O}^+]$.



However, the acid anion may play a marked role in hydration rate, eg, phosphomolybdate and phosphotungstate anions exhibit hydration rates two or three times that of sulfate or phosphate. Association of the polyacid anion with the propyl carbonium ion is suggested. Protonation of propylene occurs more readily than that of ethylene as a result of the formation of a more stable secondary carbonium ion. Thus higher conversions are achieved in propylene hydration.

There are three basic processes in commercial operation:

- Vapor-phase hydration over a fixed-bed catalyst of supported phosphoric acid (*Veba-Chemie*) or silica-supported tungsten oxide with zinc oxide promoter.
- Mixed vapor-liquid-phase hydration at low (150°C) temperature and high (10.13 MPa (100 atm)) pressure using a strongly acidic cation-exchange resin catalyst (*Deutsche Texaco AG*).
- Liquid-phase hydration at high (270°C) temperature and high (20.3 MPa (200 atm)) pressure in the presence of a soluble tungsten catalyst (*Tokuyama Soda*).

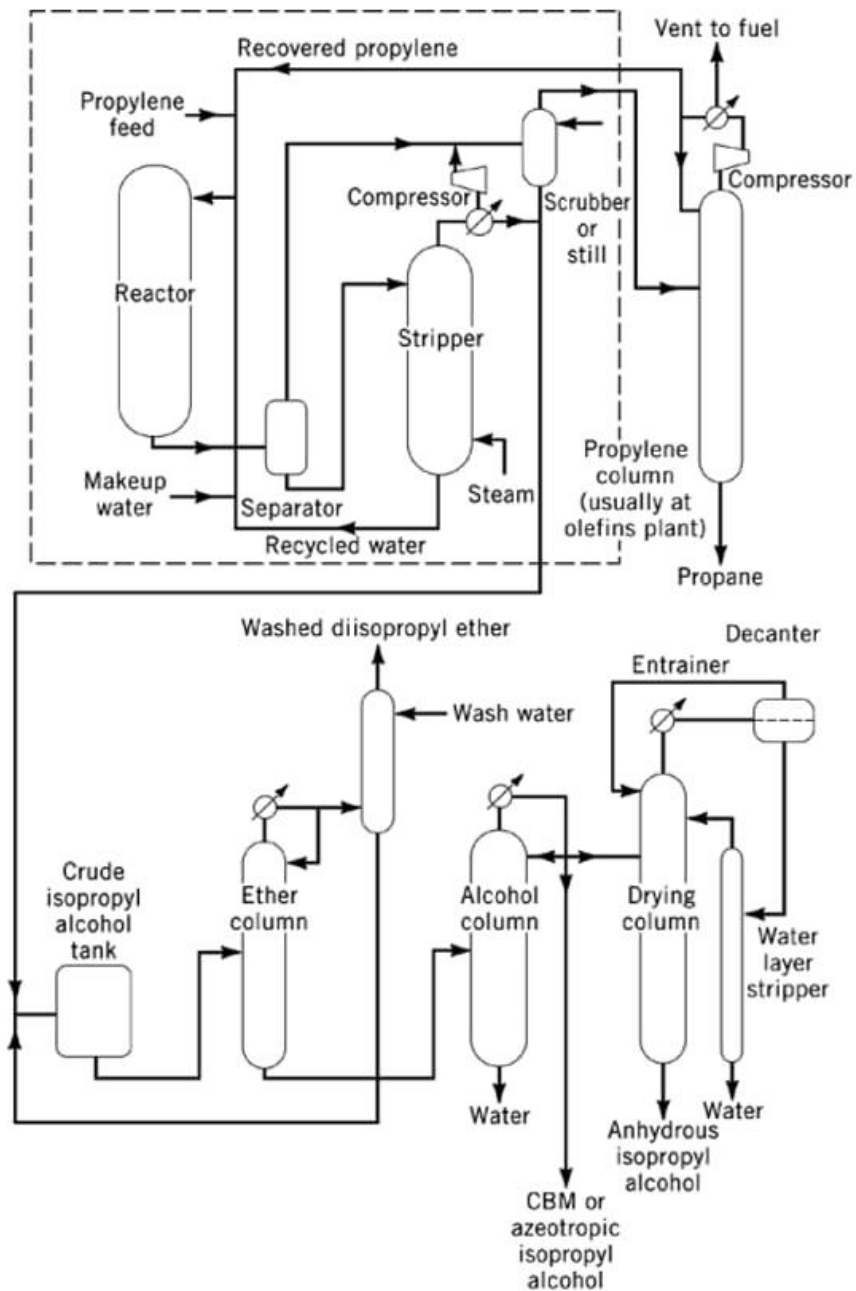


Figure 2.4 Direct hydration process for the manufacture of isopropyl alcohol ^[1]

Figure 2.4 shows us the flow chart for the direct hydration process. The description for the three direct hydration process is given below.

In the *Veba-Chemie* process, a vaporized stream of propylene and water is passed through an acidic catalyst bed (H_3PO_4 supported on SiO_2) at 240–260°C and 2.5–6.6 MPa (25–65 atm). The gas stream from the reactor is cooled and fed to a scrubber where the remaining isopropyl alcohol is removed. Isopropyl alcohol selectivity is ca 96% for the gas-phase process. Owing to equilibrium limitations in the gas phase at high temperature and low pressure, a low propylene conversion (5–6%) results and thus a large amount of unreacted propylene is recycled. Both processes involve high plant costs owing to high pressure requirements, gas recycles, and the requirement for high purity propylene (ca 99 wt %).

Deutsche Texaco developed a trickle-bed process to avoid the disadvantages of the gas-phase process. In the trickle-bed process, a mixture of liquid water and propylene gas in a molar ratio of 12 to 15:1 is introduced at the top of a fixed-bed reactor and allowed to trickle down over a sulfonic acid ion-exchange resin. Reaction between the liquid and gas phases takes place at 130–160°C and 8–10 MPa (80–100 atm), forming aqueous isopropyl alcohol. Propylene conversions per pass are greater than 75%, and isopropyl alcohol selectivity is 93%. Only 92 wt % propylene purity is needed for this process. Approximately 5% diisopropyl ether and some alcohols of the higher oligomers form as by-products. The life of the cation-exchange resin is at least eight months.

A liquid-phase variation of the direct hydration was developed by *Tokuyama Soda*. The disadvantages of the gas-phase processes are largely avoided by employing a weakly acidic aqueous catalyst solution of a silicotungstate. Preheated propylene, water, and recycled aqueous catalyst solution are pressurized and fed into a reaction chamber where they react in the liquid state at 270°C and 20.3 MPa (200 atm) and form aqueous isopropyl alcohol. Propylene conversions of 60–70% per pass are obtained, and selectivity to isopropyl alcohol is 98–99 mol % of converted propylene. The catalyst is recycled and requires little replenishment compared to other processes. The bottoms containing aqueous catalyst solution are recycled to the reactor, and the light ends are stripped of low boiling impurities, eg, diisopropyl ether and acetone. Azeotropic distillation yields dry isopropyl alcohol, and the final distillation column yields a product of more than 99.99% purity.

2.5 Detailed description of the selected process

Tokuyama Soda is the most economical and efficient process for direct hydration of propylene to isopropanol in liquid phase. The first commercial plant of this process, having a capacity of 30,000 metric tons of isopropanol per annum. In recent years, various catalysts and processes for direct hydration of propylene have been proposed. It seems necessary for a better understanding of Tokuyama Process to review some typical hydration processes briefly. The catalysts most widely proposed for the vapour-phase direct hydration of propylene are mineral acids such as phosphoric acid and heteropoly acids on silica or diatomaceous earth, and solid acids of metal oxides.

The direct hydration with a solid catalyst under a high pressure at a high mole ratio of water to propylene can be preferably employed to obtain high per pass conversions of propylene. The reaction is generally carried out by passing propylene and liquid water at a mole ratio of water to propylene between 10 and 15 over the catalyst bed at a temperature from 230 to 270°C and a pressure from 200 to 300 atm. For the hydration in the presence of liquid water, tungsten oxide is widely used as an effective component of catalyst. Tokuyama Soda has also proposed an active catalyst which comprises zirconium tungstate. This catalyst is suitable for both vapour phase and liquid-phase processes.

Catalyst System employed in Tokuyama Process essentially comprises a dilute aqueous solution of definite kinds of polytungsten compounds within a selective pH range. This catalyst system is highly active and remarkably selective for hydrating propylene to isopropanol. This system is also very stable because the catalyst components are strongly resistant to hydrolysis. Such high stability of the catalyst system is well maintained at all times in operation by the careful control of poisons which cause the decomposition of the catalyst. The catalyst life is, therefore, very long in continuous operation. Tokuyama Process gives, moreover, higher per pass conversions of propylene owing to intimate contact between dissolved propylene and the catalyst solution in the liquid phase than in the case where solid catalyst systems are employed

2.5.1 Description of the process flowsheet

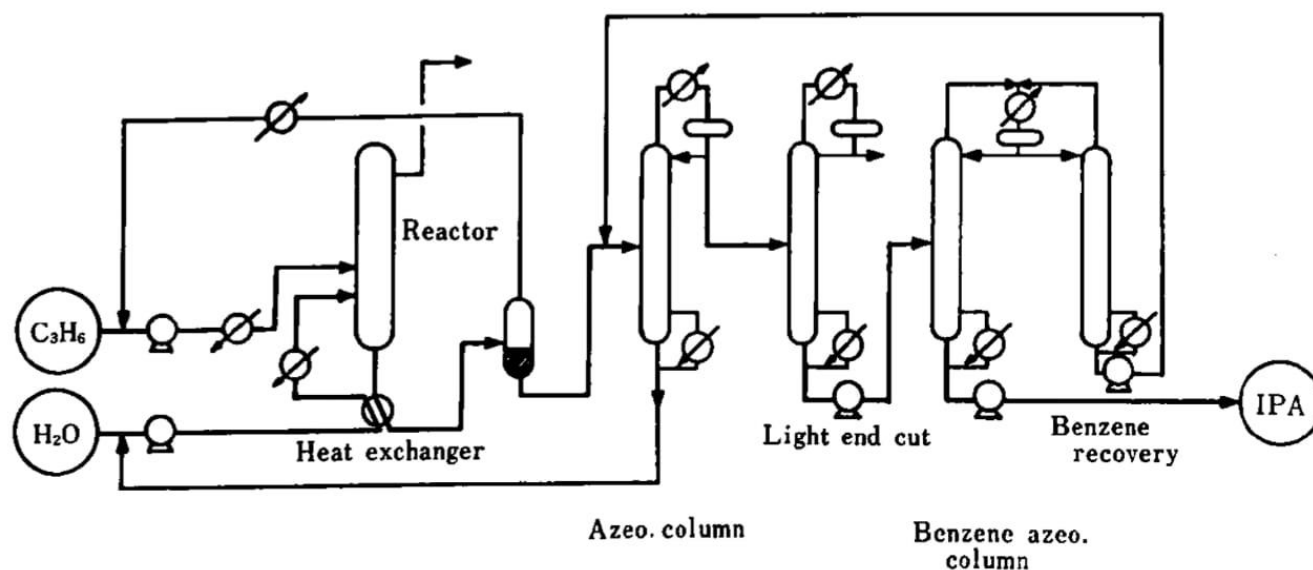


Figure 2.5 Flow diagram of Tokuyama Process for the production of isopropyl Alcohol 50 tons/day ^[5]

Figure 2.5 is the flow diagram for the Tokuyama process where liquid propylene is preheated and fed to a reactor under pressure. The catalyst solution recovered from the azeotrope column is preheated by heat exchange with the reactor effluent and fed to the reactor operating at $240\sim 270^{\circ}\text{C}$ and $150\sim 250\text{atm}$. The reaction takes place in the liquid phase between dissolved propylene and water. The aqueous solution containing isopropanol and catalyst is withdrawn from the reactor and cooled by heat exchange and then flashed under reduced pressure in a gas separator where the unconverted propylene dissolved in the solution is separated and recycled.

The liquid is sent to the azeotropic column, from where azeotropic mixture of isopropanol and water is drawn off and sent to further distillation steps for purification and dehydration. The aqueous solution containing catalyst from the bottom of the azeotrope column joins with fresh water and is recycled to the reactor. The azeotrope alcohol is freed of the light impurities in the first rectifying column and then dehydrated in two further columns with benzene as the dehydrating agent. To obtain a high grade isopropanol (99.99% purity), another additional distillation step is necessary. Under the optimum reaction conditions, the range of propylene conversion per pass is about $60\sim 70\%$ and selectivity to isopropanol based on the converted

propylene is as much as 98~ 99%. The major by-product is di-isopropyl ether. In Tokuyama Process, both the spent gas from the reactor and all the by-products drawn off at the purification section are completely utilized as fuel for heating in the system.

2.5.2 Novelty of the process

Tokuyama Process has a number of advantages based on its own catalyst system and process design. The features of the process confirmed in commercial operation are as follows:

- The catalyst system comprises a homogeneous dilute aqueous solution which maintains high activity and excellent selectivity for hydrating propylene to isopropanol.
- The catalyst solution is so highly stabilized that it is circulated repeatedly in the reaction system without any additional treatments. Catalyst life is, therefore, very long.
- Since the reaction is carried out in aqueous solution under high pressure, the formation of isopropanol is favoured by equilibrium effect.
- 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. Commercial propylene of about 95% concentration is normally used.
- The amount of by-products is remarkably small because the reaction takes place in an aqueous solution of highly selective catalyst. Organic acids and aldehydes are hardly detectable in the reaction product. A high grade isopropanol is easily obtained at the purification section.
- Since the reaction is carried out in aqueous solution, the heat loss incidental to evaporation and condensation of water can be avoided.
- Because of absence of corrosion in the system, easy operation and maintenance of equipments are possible.
- 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

Thermodynamic feasibility studies are conducted to predict whether a chemical reaction is feasible at a given temperature and pressure. Gibbs free energy is a parameter used to determine the feasibility of a reaction. Gibbs free energy when negative, indicates that the reaction is feasible at a given temperature and pressure, otherwise (when positive) the reaction is not feasible and will require changes in temperature/pressure in order to promote the reaction.

Gibbs free energy is calculated using the following relation

$$\Delta G_{\text{reaction}} = \Sigma (G_f)_{\text{products}} - \Sigma (G_f)_{\text{reactants}}$$

Reactions involved:

1. $\text{CH}_3\text{CH}=\text{CH}_2 + \text{H}_2\text{O} \rightleftharpoons (\text{CH}_3)_2\text{CHOH}$
2. $2(\text{CH}_3)_2\text{CHOH} \rightleftharpoons \text{H}_2\text{O} + [(\text{CH}_3)_2\text{CH}]_2$

Thermodynamic properties of compounds are shown in table 3.1.

Table 3.1 Thermodynamic Properties of Compounds

COMPOUNDS	$\Delta H_f(\text{kJ/mol})$	$\Delta G_f(\text{kJ/mol})$
$\text{CH}_3\text{CH}=\text{CH}_2$	20.41	62.22
$\text{H}_2\text{O}(\text{liq})$	-285.83	-228.374
$(\text{CH}_3)_2\text{CHOH}$	-306.3	-162.44
$[(\text{CH}_3)_2\text{CH}]_2\text{O}$	-318.70	-164.88

Equations used:

1. $\Delta G_{\text{reaction}} = \Sigma (G_f)_{\text{products}} - \Sigma (G_f)_{\text{reactants}}$
2. $\Delta H_{\text{reaction}} = \Sigma (H_f)_{\text{products}} - \Sigma (H_f)_{\text{reactants}}$
3. $\Delta G = -RT \ln(K)$
4. $\ln\left(\frac{K_1}{K_2}\right) = -\frac{\Delta H}{RT} \left[\frac{1}{T_2} - \frac{1}{T_1}\right]$ (Vant Hoff equation)

The feasibility studies of the reactions are shown as follows

3.1 Reaction 1 (Reaction temperature = 523K)

Enthalpy of reaction at room temperature

$$\begin{aligned}\Delta H_{\text{reaction}} &= \sum \Delta H_{\text{products}} - \sum \Delta H_{\text{reactants}} \\ &= [-306.3 - (-285.83 + 20.41)] \\ &= -40.88 \text{ kJ/mol}\end{aligned}$$

Gibbs free energy at room temperature

$$\begin{aligned}\Delta G_{\text{reaction}} &= \sum \Delta G_{\text{products}} - \sum \Delta G_{\text{reactants}} \\ &= [-162.44 - (62.22 - 228.374)] \\ &= 3.714 \text{ kJ/mol}\end{aligned}$$

Using Gibbs free energy equation

$$\Delta G = -RT \ln(K)$$

$$\ln K = -\Delta G/RT$$

Where $R = 0.008314 \text{ kJ/mol}\cdot\text{K}$ and $T = 298\text{K}$

$$\ln K_1 = (-3.714)/(0.008314 \times 298)$$

$$\ln K_1 = 1.4982$$

Using Vant Hoff equation, we get

$$\ln\left(\frac{K_1}{K_2}\right) = -\frac{\Delta H}{RT} \left[\frac{1}{T_2} - \frac{1}{T_1}\right]$$

$$\ln\left(\frac{K_1}{K_2}\right) = -\frac{-(-40.88)}{0.008314} \left[\frac{1}{523} - \frac{1}{298}\right]$$

$$\ln K_2 = 5.5946$$

$$\Delta G = -RT \ln(K)$$

$$\Delta G = -(0.008314 \times 523 \times 5.5946)$$

$$\Delta G = -24.3335 \text{ kJ/mol}$$

Since $\Delta G_{\text{reaction}} < 0$, the reaction is feasible at reaction temperature

Therefore, reaction 1 is thermodynamically feasible.

3.2 Reaction 2 (Reaction temperature =523K)

Enthalpy of reaction at room temperature

$$\begin{aligned}\Delta H_{\text{reaction}} &= \sum \Delta H_{\text{products}} - \sum \Delta H_{\text{reactants}} \\ &= [-285.33 - 318.70 - (2x - 306.3)] \\ &= 8.57 \text{ kJ/mol}\end{aligned}$$

Gibbs free energy at room temperature

$$\begin{aligned}\Delta G_{\text{reaction}} &= \sum \Delta G_{\text{products}} - \sum \Delta G_{\text{reactants}} \\ &= [-228.374 - 164.88 - (2x - 162.44)] \\ &= -68.374 \text{ kJ/mol}\end{aligned}$$

Using Gibbs free energy equation

$$\Delta G = -RT \ln(K)$$

$$\ln K = -\Delta G/RT$$

Where $R = 0.008314 \text{ kJ/mol}\cdot\text{K}$ and $T = 298\text{K}$

$$\ln K_1 = -(-68.374)/(0.008314 \times 298)$$

$$\ln K_1 = 27.5832$$

Using Vant Hoff equation, we get

$$\ln\left(\frac{K_1}{K_2}\right) = -\frac{\Delta H}{RT} \left[\frac{1}{T_2} - \frac{1}{T_1}\right]$$

$$\ln\left(\frac{K_1}{K_2}\right) = -\frac{-8.57}{0.008314} \left[\frac{1}{523} - \frac{1}{298}\right]$$

$$\ln K_2 = 26.0962$$

$$\Delta G = -RT \ln(K)$$

$$\Delta G = -(0.008314 \times 523 \times 26.0962)$$

$$\Delta G = -113.5046 \text{ kJ/mol}$$

Since $\Delta G_{\text{reaction}} < 0$, the reaction is feasible at reaction temperature

Therefore, reaction 2 is thermodynamically feasible

Material balances play a major role in designing a process plant. In a process, it is necessary that material balance is studied for the overall process and for individual equipments in order to determine the amount of raw materials required to run the process, compositions of each streams and the flow rates of each steam. Here, material balance is studied for the production of 50 tons/day of Isopropyl alcohol. The material balance is conducted for the entire plant and for individual equipments. Henceforth, all flow rates will be depicted in kmol/h

4.1 Production Rate

50 tons of Isopropyl alcohol is produced every day

2083.333 kg of Isopropyl alcohol is produced every hour

Therefore, 2083.333 kg/hr of Isopropyl alcohol is produced.

4.2 Raw Material Requirement

From stoichiometry, to produce 2083.33 kg/hr Isopropyl alcohol, i.e.34.967kmol/hr we will require exactly the same amount of propylene and water (feed).

Therefore, 34.967 kmol/hr of propylene and water is required as raw material.

Water is fed in 1:1 ratio to propylene

Amount of water required = $34.967 \times 1 = 34.967$ kmol/hr

Therefore, 34.967 kmol/hr of air is required.

4.3 Material balance across individual equipments

4.3.1 Material balance across Reactor



Figure 4.1 Reactor with inlet and outlet streams used in the manufacture of isopropyl alcohol 50 tons/day

Figure 4.1 Shows the inlet and outlet material stream of a reactor

Weight of $\text{CH}_3\text{CH}=\text{CH}_2$ entering = 34.967 kmol/hr

Weight of H_2O entering = 34.967 kmol/hr

Reaction occurring: $\text{CH}_3\text{CH}=\text{CH}_2 + \text{H}_2\text{O} \longrightarrow (\text{CH}_3)_2\text{CHOH}$

Amount of $\text{CH}_3\text{CH}=\text{CH}_2$ recycled = 10.4901 kmol/hr

Amount of $\text{CH}_3\text{CH}=\text{CH}_2$ entering the reactor = 45.95286 kmol/hr

Moles of H_2O entering = 34.967 kmol/hr

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

Amount of $(\text{CH}_3)_2\text{CHOH}$ formed = $0.7 \times (45.9586)$ kmol of $\text{CH}_3\text{CH}=\text{CH}_2$

= 34.967 kmol of $(\text{CH}_3)_2\text{CHOH}$

Amount of H_2O formed = 0.3×34.967 kmol H_2O

= 10.4901 kmol of H_2O

Table 4.1 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

Table 4.1 gives us the result for the material balance which was conducted across a reactor

4.3.2 Material Balance across Heat Exchanger



Figure 4.2 Heat Exchanger with inlet and outlet streams used in the manufacture of isopropyl alcohol
50 tons/day

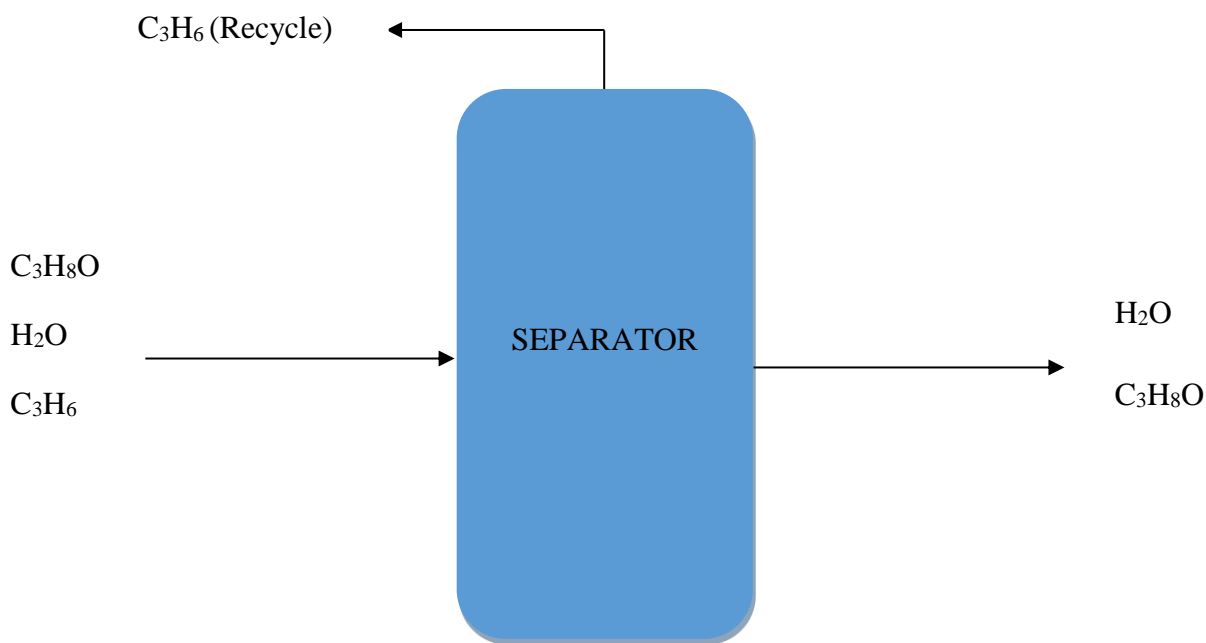
Figure 4.2 shows the inlet and outlet material streams of the heat exchanger.

Table 4.2 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

Table 4.2 gives us the result of the material balance which was conducted across a heat exchanger

4.3.3 Material Balance across Separator



**Fig 4.3 Separator with inlet and outlet streams used in the manufacture of isopropyl alcohol
50 tons/day**

Figure 4.3 shows us the inlet and outlet steam of a separator

Amount of C_3H_6 entering= 14.98586 kmol/hr

Amount of C_3H_6 Recycled=14.98586kmol/hr

Amount of C_3H_6 leaving = 0 kmo/hr

Table 4.3 Material balance across separator

Compounds	Material entering (kmol/h)	Recycle (kmol/h)	Material leaving (kmol/h)
Propylene	14.9859	14.9859	0
Water	14.9859	0	14.9859
Isopropyl Alcohol	34.967	0	34.967
Total	64.9387	14.9859	49.9528

Table 4.3 gives us the result for the material balance which was conducted across a separator

4.3.4 Material balance across Distillation Column

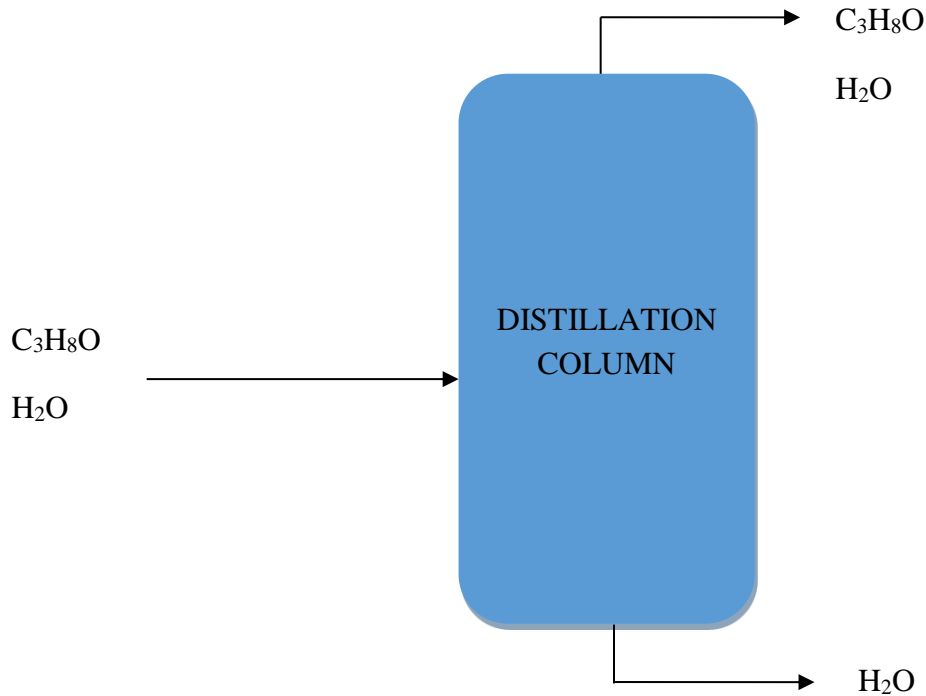


Figure 4.4 Distillation column with inlet and outlet streams used in the manufacture of isopropyl alcohol 50 tons/day

Figure 4.4 shows the inlet and outlet material stream of a distillation column

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

Amount of H_2O entering = 10.4901 kmol/hr

Amount of $\text{C}_3\text{H}_8\text{O}$ entering = 34.967 kmol/hr

Moles of H_2O leaving (top) = 0.01×34.967

= 0.3496 kmol/hr

Amount of $\text{C}_3\text{H}_8\text{O}$ Leaving (top) having 99% purity = 34.967 kmol/hr

Amount of H_2O leaving the bottom stream = 10.14043 kmol/hr

Table 4.4 Material balance across distillation column

Compounds	Material entering (kmol/h)	Top stream (kmol/h)	Bottom stream (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

Table 4.4 gives us the result of the material balance which was conducted across a distillation column

4.4 Overall Material Balance

The material balance across the entire process is shown in table 4.5.

Table 4.5 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

As with mass, energy can be considered to be separately conserved in all but nuclear processes. In process design, energy balances are made to determine the energy requirements of the process: the heating, cooling and power required.

The steady state energy balance is generally calculated using the relation:

Energy out=Energy in + Heat of Reaction + Q (heat supplied/heat removed)

In this section, we estimate the amount of utilities (coolant and duty) required by the plant for the production of 50 tons/day of Isopropyl Alcohol. Accordingly, enthalpy balance is performed over individual equipments, assuming heat losses to be negligible and all pumps and compressors to neither supply nor dissipate heat.

5.1 Reactor

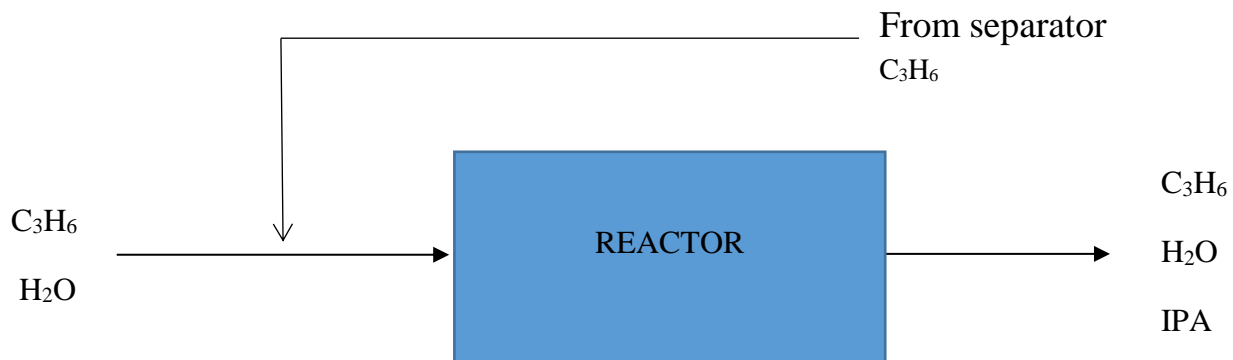


Figure 5.1 Reactor with inlet and outlet streams used in the manufacture of isopropyl alcohol 50 tons/day
Figure 5.1 shows us the inlet and outlet energy streams across of a reactor

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

$$P_1 = 1 \text{ atm}$$

$$P_2 = 200 \text{ atm}$$

$$R = 0.0821 \text{ L.atm/K.mol}$$

$$C_p = 84.5495$$

$$T_2 = 250^\circ \text{ C}$$

$$T_2/T_1 = (P_2/P_1)^{(R/C_p)}$$

$$T_1 = (250) \times (1/200)^{(84.5495/0.0821)}$$

$$T_1 = 246^\circ \text{ C}$$

Table 5.1 Energy balance for reactor

	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 ₃ H ₆	49.95286	131.0667	519	445.5704	14.98586	131.733	523	137.0925
H ₂ O	49.95286	90.666	519	308.2254	14.98586	90.666	523	95.47286
IPA	-	-	-	-	34.967	375.4043	523	899.6766
	TOTAL			753.7958	TOTAL			1132.248

Table 5.1 shows the energy balance performed across a reactor

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

Table 5.2 Total energy balance for reactor

	TOTAL ENERGY ENTERING (kJ/s)	TOTAL ENERGY LEAVING (kJ/s)
Reactants enthalpies	753.79588	-
Products enthalpies	-	1132.248
Heat of reaction	378.4521	-
Heat transferred	-	-
TOTAL	1132.248	1132.248

Table 5.2 shows the total energy entering and leaving the reactor

5.2 Heat exchanger



Figure 5.2 Heat exchanger with inlet and outlet streams used in the manufacture of isopropyl alcohol 50 tons/day

Table 5.3 Energy balance for heat exchanger

	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 ₃ H ₆	14.98586	131.733	523	137.0925	14.98586	103.733	313	158.0113
H ₂ O	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	TOTAL			236.2651

Table 5.3 shows the energy balance performed across a heat exchanger

From energy balance equation,

Total Energy Leaving= Total Energy Entering

Energy Out = Energy In + Heat of Reaction + Q

$$236.2651=1144.152+0+Q$$

$$Q = -907.8869/s$$

Heat transferred out of the product mixture to cool the gases to a temperature of 40° C and subsequently generate liquid is 907.8869kJ/s

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

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

$$907.8869= [mC_{p1} (T_2-T_1) + m \lambda + mC_{p2} (T_3-T_2)]$$

$$907.8869 = m \cdot [75.766 \cdot (273 - 283) + 40680 + 76.32 \cdot (383 - 273)]$$

$$m = 0.0211 \text{ kmol/s}$$

$$m = 76.2792 \text{ kmol/h}$$

Mass of chilled water (coolant) required to cool down the gases is 76.2792 kmol/h

Table 5.4 Total energy balance for heat exchanger

	TOTAL ENERGY ENTERING (kJ/s)	TOTAL ENERGY LEAVING (kJ/s)
Inlet energy	1144.152	-
Outlet energy	-	236.2651
Heat of reaction	-	-
Heat transferred	-	907.8869 (cooling)
TOTAL	1144.152	1144.152

Table 5.3 shows the total energy entering and leaving the Heat exchanger

5.3 Condenser

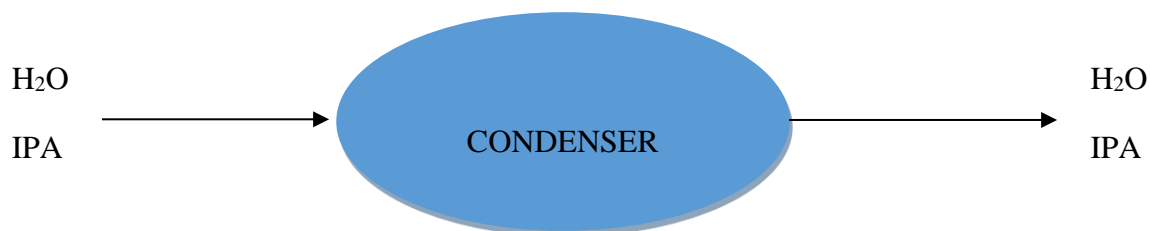


Figure 5.3 Condenser with inlet and outlet streams used in the manufacture of isopropyl alcohol 50 tons/day

Table 5.5 Energy balance for 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 ₂ O	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

Table 5.5 shows the energy balance performed across a condenser

From energy balance equation,

Total Energy Leaving= Total Energy Entering

Energy Out = Energy In + Heat of Reaction + Q

$$48.31508 = 191.7005 + 0 + Q$$

$$Q = -143.385 \text{ kJ/s}$$

Heat transferred out of the product mixture to cool the vapours to a temperature of 30° C and subsequently generate liquid is 143.385 kJ/s

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

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

$$143.385 = mC_{p1} (T_2 - T_1)$$

$$143.385 = m * [75.366 * (333 - 283)]$$

$$m = 0.03805 \text{ kmol/s}$$

$$m = 136.9814 \text{ kmol/h}$$

Mass of chilled water (coolant) required to cool down the gases is 76.2792 kmol/h

Table 5.6 Total energy balance for condenser

	TOTAL ENERGY ENTERING (kJ/s)	TOTAL ENERGY LEAVING (kJ/s)
Inlet energy	191.7005	-
Outlet energy	-	48.31508
Heat of reaction	-	-
Heat transferred	-	143.385 (Condensation)
TOTAL	191.7005	191.7005

Table 5.6 shows the total energy entering and leaving the condenser

5.4 Reboiler

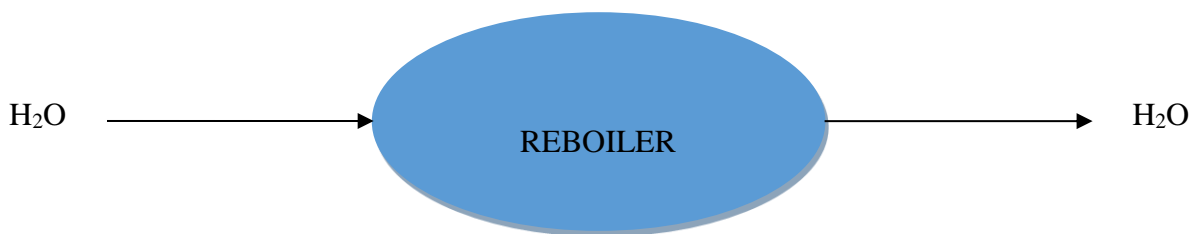


Figure 5.4 Reboiler with inlet and outlet streams used in the manufacture of isopropyl alcohol 50 tons/day

Table 5.7 Energy balance for 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 ₂ O	10.14043	75.312	333	12.72826	10.14043	75.7224	378	22.3958
	TOTAL			12.72826	TOTAL			22.3958

Table 5.7 shows the energy balance performed across a reboiler

From energy balance equation,

Total Energy Leaving = Total Energy Entering

Energy Out = Energy In + Heat of Reaction + Q

$$22.3958 = 12.72826 + 0 + Q$$

$$Q = 9.6674 \text{ kJ/s}$$

$$\text{Reboiler duty} = 9.6674 \text{ kW}$$

Table 5.8 Total energy balance for reboiler

	TOTAL ENERGY ENTERING (kJ/s)	TOTAL ENERGY LEAVING (kJ/s)
Inlet energy	12.72826	-
Outlet energy	-	22.3958
Heat of reaction	-	-
Heat transferred	9.6674	-
TOTAL	22.3958	22.3958

Table 5.8 shows the total energy entering and leaving the reboiler

The design of equipment mainly deals with studying the design parameters and specifications of each equipment involved in the manufacturing process. This chapter discusses about process and mechanical design of equipments used in the production of Isopropyl alcohol.

6.1 Reactor design

The reactor here is a CSTR. Propylene on reaction with water yields Isopropyl alcohol.

$$K = 0.00623 \text{ s}^{-1} \text{ [6]}$$

For a CSTR performance equation is given by, $\tau = C_{ao}X_a/-r_a$

Reactor pressure = 200 atm

Residence time (τ) = 0.1 hours

Volumetric flow rate of the reactant mixture = 23.3891 m³/h

Total Volume of reactor (V) = $V_o \times \tau$

$$= 0.1 \times 23.3891$$

$$= 2.3891 \text{ m}^3$$

Considering free space of 10%

Total volume = 2.3891 + (0.1 × 2.3891)

$$= 2.62801 \text{ m}^3$$

Mechanical Design

Number of baffles = 4

Number of Impeller blades = 6

Assuming $H/D = 2$

Substituting in $V = 3.14 (D^2/4) \times H$, where $H = 2 D$

We get Diameter of the reactor, $D_m = 1.1873 \text{ m}$

Height of the reactor $H = 2.3746 \text{ m}$

Diameter of the Impeller, $D_{\text{imp}} = 40 \% D_m = 0.4749 \text{ m}$

Baffle thickness $= D_m / 12 = 0.0989 \text{ m}$

Height of Impeller blade, $h = 20 \% D_m = 0.2374 \text{ m}$

Width of Impeller blade, $w = 25 \% D_m = 0.296825 \text{ m}$

Bottom clearance, $E = D_m / 3 = 0.3957 \text{ m}$

Wall thickness, $t = \frac{P \times D}{200 \times f \times J - P} + C$ (IS 2825)

Where,

t = thickness in mm

P = operating pressure in kgf/cm^2 ($1 \text{ atm} = 1.0332 \text{ kgf/cm}^2$)

D = diameter of column in mm (1254 mm)

f = allowable stress (13)

J = joint efficiency (0.85)

C = corrosion allowance (min 5 mm)

$$t = \frac{200 \times 1.032 \times 1187.3}{(200 \times 13 \times 0.85) - 200 \times 1.0332} + 5 = 122.31 \text{ mm}$$

The thickness of the reactor is 12.231 cm

Outer diameter $D_o = \text{inner diameter} + \text{thickness}$

$$D_o = 1187.3 + 122.31 = 1309.61 \text{ mm}$$

Assuming Torispherical head,

$$\text{Crown radius, } r_c = 0.9 \times D_o = 0.9 \times 1309.61 = 1178.649 \text{ mm}$$

Knuckle radius, $r_k = 0.17 \times D_m = 0.17 \times 1187.3 = 201.841$ mm

6.2 Heat exchanger design

Heat exchanger is used to remove excess heat from the product stream (Propene, IPA and H₂O). It is a Double pipe heat exchanger where water is used as the cooling medium

Table 6.1 Inlet and outlet flow streams of heat exchanger used in the manufacture of Isopropyl alcohol

	Inlet Temp. (°C)	Outlet Temp. (°C)	Mass flow rate, (kg/s)	T _{avg} (°C)
Hot fluid	250	40	0.81	145
Cold fluid	10	110	0.3798	60

Table 6.1 shows the temperatures of inlet and outlet streams of heat exchanger

Table 6.2 Properties of Streams at average temperature

Property	Product Mixture	Water
Specific Heat, C _p (kJ/kg-K)	3.814	4.184
Density, ρ (kg/m ³)	628.42	983.2
Thermal Conductivity, k(W/m-K)	0.0882	0.358
Viscosity, μ (kg/m-s)	0.0002125	0.000478

From heat balance the mass flow rate of cold fluid was found to be = 0.3798 kg/s

Table 6.2 gives the properties of the product mixture and water at average temperature

Table 6.3 Pipe Dimensions

Outer diameter of outer pipe, D _o	0.06 m
Inner diameter of outer pipe, D _i	0.052 m
Outer diameter of inner pipe, d _o	0.0421 m
Inner diameter of inner pipe, d _i	0.03505 m
Standard Length of Pipe, L _r	4.5 m

Table 6.3 shows the standard pipe dimensions

Logarithmic Mean Temperature Difference Calculations

$$LMTD = \frac{(Thi - Tco) - (Tho - Tci)}{\ln \frac{(Thi - Tco)}{(Tho - Tci)}}$$

Log mean temperature, $\Delta T_{LMTD} (^{\circ}C) = 71.407^{\circ}C$

Inner side and annular side heat transfer coefficient calculations

Table 6.4 Inner side heat transfer properties

Flow area	$A = (\pi/4) \times d_i^2$	0.000964 m ²
Mass velocity	$G = m / A$	839.922 kg/ m ² -s
Reynolds number	$N_{Re} = (d_{ix}G)/\mu$	138549.268
Prandtl number	$N_{Pr} = (C_p \times \mu)/k$	9.18
Nusselt number	$N_{Nu} = 0.023 \times Re^{0.8} \times Pr^{0.33}$	610.816
Inside heat transfer coefficient	$h_i = N_{Nu} \times k / d_i$	1537.0605 W/m ² -C ⁰

Table 6.4 shows the calculations for inner heat transfer coefficient

Table 6.5 Annular side heat transfer properties

Equivalent diameter	$D_e = (D_i^2 - d_o^2) / d_o$	0.02218 m
Flow area	$A = (\pi/4) \times (D_i^2 - d_o^2)$	0.000731 m ²
Mass velocity	$G = m / A$	519.350 kg/ m ² -s
Reynolds number	$N_{Re} = (D_{ex}G)/\mu$	24098.709
Prandtl number	$N_{Pr} = (C_p \times \mu)/k$	5.58
Nusselt number	$N_{Nu} = 0.023 \times Re^{0.8} \times Pr^{0.4}$	146.546
Annular heat transfer coefficient	$h_o = N_{Nu} \times k / D_e$	2365.350 W/m ² -C ⁰

Table 6.4 shows the calculations for annular heat transfer coefficients

Table 6.6 Overall heat transfer coefficient

Dirt factor	R_D	$0.000705\text{m}^2\text{-C}^0/\text{W}$
$1/U$	$(1/h_i) + (1/h_o) + R_D$	$0.00177836\text{ m}^2\text{-C}^0/\text{W}$
Overall heat transfer coefficient	U	$523.764\text{W}/\text{m}^2\text{-C}^0$

Table 6.6 shows the calculations for overall heat transfer coefficient

Number of tubes and hairpin bends

From energy balance excess heat to be removed from product stream is,

$$Q = 1023.7 \text{ kW}$$

Table 6.7 Number of tubes and hairpin bends

Heat transfer area	$A = Q/(U \times \Delta T_{LMTD})$	27.3713 m^2
Number of tubes	$N_t = A/(\pi d_o L_r)$	46
Number of hairpin bends	$N_b = N_t - 1$	45

Table 6.7 shows the number of hair pin bends required in the distillation column

Mechanical Design

$$\text{Wall thickness, } t = \frac{P \times D}{200 \times f \times J - P} + C \text{ (IS 2825)}$$

Where,

t = thickness in mm

P = operating pressure in kgf/cm^2 ($1 \text{ atm} = 1.0332 \text{ kgf}/\text{cm}^2$)

D = diameter of column in mm (60 mm)

f = allowable stress (13)

J = joint efficiency (0.85)

C = corrosion allowance (min 5 mm)

$$t = \frac{1 \cdot 1.032 \cdot 60}{(200 \times 13 \times 0.85) - 1.0332} + 5 = 5.028 \text{ mm}$$

The thickness of the heat exchanger is 5.028 mm

6.3 Distillation column design

Distillation process is carried out to increase the purity of Isopropyl alcohol to 99%.

Table 6.8 Stream composition of distillation column in terms of IPA

Feed composition, x_F	0.769
Distillate composition, x_D	0.99
Bottom composition, x_w	0.03

Table 6.8 shows the feed composition in the distillation column

To calculate number of stages

Feed temperature = 40°C = 313 K

Table 6.9 Relative volatility

Vapour pressure of IPA (mm of Hg)	$\ln P_{IPA}^V = 16.6796 - 3640.2/(-53.5+313)$	14.149
Vapour pressure of H ₂ O (mm of Hg)	$\ln P_w^V = 16.3872 - 3885.7/(-42.9+313)$	7.396
Relative volatility, α	$\alpha = P_{IPA}^V / P_w^V$	1.913

Table 6.9 shows the relative volatility calculations

Equilibrium relation is given by,

$$y^* = \alpha x / (1 + x(\alpha - 1))$$

Table 6.10 gives the equilibrium data calculated using Raoult's law

Table 6.10 Equilibrium data

x	y
0	0
0.03	0.056
0.126	0.215
0.222	0.35
0.318	0.468
0.414	0.576
0.51	0.666
0.606	0.746
0.702	0.817
0.798	0.878
0.894	0.942
0.99	0.997

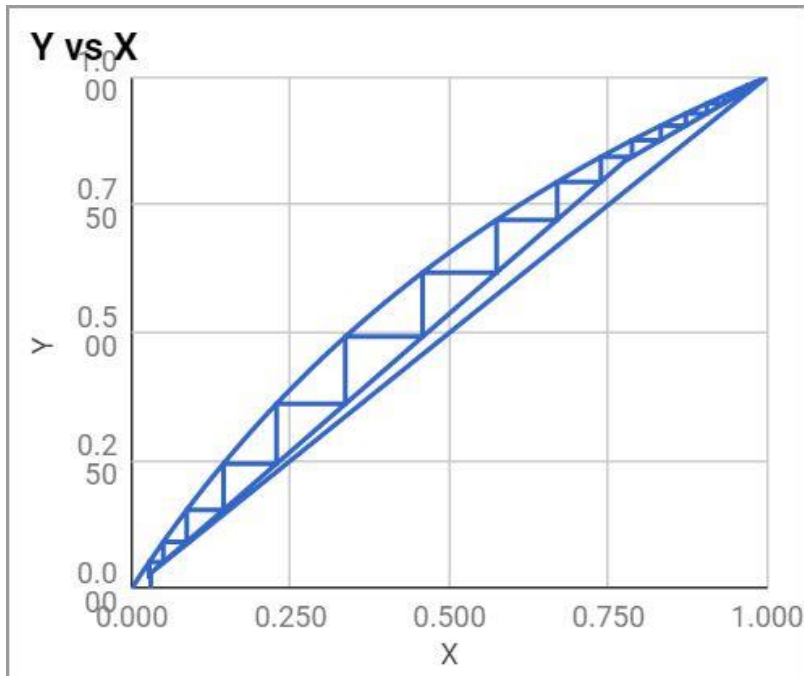


Figure 6.1 plot of y vs x for R_{actual}

Figure 6.1 shows plot of y vs x for R_{actual}

Since feed is sent at a temperature below boiling point it is subcooled liquid.

For subcooled liquid q is given by,

$$q = (C_{pf}X(T_b - T_f) + \lambda_f) / \lambda_f$$

$$q = (103.06x(82.3 - 40) + 45900) / 45900$$

$$q = 1.1$$

$$\text{slope of } q\text{-line} = q / (q - 1)$$

$$q / (q - 1) = 1.1 / (1.1 - 1) = 11$$

From graph of y vs x to determine R_m , rectification line intersects y-axis at $x_D / (R_m + 1)$

$$x_D / (R_m + 1) = 0.43$$

$$\text{Minimum reflux ratio, } R_m = (x_D / 0.43) - 1 = (0.99 / 0.43) - 1 = 1.3$$

$$R_m = 1.3$$

$$\text{Actual reflux ratio, } R_{\text{actual}} = 2 \times R_m = 2 \times 1.3 = 2.6$$

$$R_{\text{actual}} = 2.6$$

$$\text{Number of ideal stages} = 17.8$$

$$\text{Assuming efficiency, } \eta = 0.6$$

$$\text{Number of actual stages} = \text{number of ideal stages} / \eta = 17.8 / 0.6 = 29.66 \approx 30$$

$$\text{Number of actual stages} = 30$$

$$\text{Feed plate location} = 12$$

To calculate height of column

Height of column, $H = (\text{Number of stages} \times \text{Tray spacing}) + \text{Topcomer height} + \text{Downcomer height}$

Assume,

$$\text{Tray spacing} = 18 \text{ inches} = 450 \text{ mm}$$

$$\text{Topcomer height} = \text{Downcomer height} = 500 \text{ mm}$$

$$H = (30 \times 450) + 500 + 500 = 14500 \text{ mm}$$

$$H = 14.5 \text{ m}$$

To calculate diameter of column

Table 6.11 Properties of Distillation column fluids

Boiling point of IPA	82.3°C
Boiling point of water	100°C
Molecular weight of IPA	60

Molecular weight of water	18
Operating pressure	1 atm
Reflux ratio	2.6
Feed flowrate, F	45.4571 kmol/h
Distillate flowrate, D	34.967 kmol/h
Bottom flowrate, W	10.49043 kmol/h

Table 6.11 gives us the properties of the distillation column fluids

Table 6.12 Calculation of Enriching section diametre

Liquid flowrate, L	$L = RxD$	90.9142kmol/h
Gas flowrate, G	$G = L + D$	125.8812kmol/h
Density of gas, ρ_g	$\rho_g = (P \times M) / (R \times T)$	2.0442 kg/m ³
Density of liquid, ρ_L	$\rho_L = \rho_{IPAXD} + \rho_{WX} (1 - x_D)$	787.546 kg/m ³
F_{LV}	$F_{LV} = (L/G) \times (\rho_g / \rho_L)^{0.5}$	0.0367
C_{SB}	From C_{SB} vs F_{LV} plot	0.28
U_{nf}	$U_{nf} = C_{SB} / (\rho_g / (\rho_L - \rho_g))^{0.5}$	1.6729 m/s
Operating velocity, U_n	$U_n = 0.7 \times U_{nf}$	1.17103 m/s
Volumetric flowrate, Q	$Q = (G \times M) / (3600 \times \rho_g)$	1.0191 m ³ /s
Area, A	$A = Q / U_n$	0.8702 m ²
Area to be considered, A_T	$A_T = A / 0.88$	0.9889 m ²
Diameter, D_T	$D_T = ((4 \times A_T) / \pi)^{0.5}$	1122.383 mm

Table 6.4 shows the calculations for enriching section diameter

Table 6.13 Calculation of Stripping section diametre

Liquid flowrate, L'	$L' = L + qF$	140.917 kmol/h
Gas flowrate, G'	$G' = L' - W$	130.426 kmol/h
Density of gas, ρ_g	$\rho_g = (P \times M) / (R \times T)$	0.6608 kg/m ³
Density of liquid, ρ_L	$\rho_L = \rho_{IP} \times x_w + \rho_w \times (1 - x_w)$	993.562 kg/m ³
F_{LV}	$F_{LV} = (L/G) \times (\rho_g / \rho_L)^{0.5}$	0.027
C_{SB}	From C_{SB} vs F_{LV} plot	0.28
U_{nf}	$U_{nf} = C_{SB} / (\rho_g / (\rho_L - \rho_g))^{0.5}$	3.29 m/s
Operating velocity, U_n	$U_n = 0.7 \times U_{nf}$	2.303 m/s
Volumetric flowrate, Q	$Q = (G \times M) / (3600 \times \rho_g)$	1.0559 m ³ /s
Area, A	$A = Q / U_n$	0.4584 m ²
Area to be considered, A_T	$A_T = A / 0.88$	0.5209 m ²
Diameter, D_T	$D_T = ((4 \times A_T) / \pi)^{0.5}$	814.596 mm

Table 6.4 shows the calculations for stripping section diameter

Since the diameter of enriching section is more than that of stripping section, we consider the diameter of the column to be 1122.383 mm.

$$\text{Wall thickness, } t = \frac{P \times D}{200 \times f \times J - P} + C \text{ (IS 2825)}$$

Where,

t = thickness in mm

P = operating pressure in kgf/cm² (1 atm = 1.0332 kgf/cm²)

D = diameter of column in mm (1122.383 mm)

f = allowable stress (13)

J = joint efficiency (0.85)

C = corrosion allowance (min 10 mm)

$$t = \frac{1 \cdot 1.032 \cdot 1122.383}{(200 \times 13 \times 0.85) - 1.0332} + 10 = 10.5243 \text{ mm}$$

The thickness of the distillation column is 10.5243 mm

6.4 Condenser Design

The condenser cools the product gases to room temperature. It is a shell and tube heat exchanger where water is used as the cooling fluid. Table 6.14 shows the inlet and outlet temperatures of product mixture (hot fluid) and water (cold fluid)

Table 6.14 Inlet and outlet flow streams of condenser used in the manufacture of Isopropyl alcohol

	Inlet Temp. ($^{\circ}\text{C}$)	Outlet Temp. ($^{\circ}\text{C}$)	Mass flow rate, (kg/s)	T_{avg} ($^{\circ}\text{C}$)
Hot fluid	90	50	0.582783	70
Cold fluid	10	60	0.68605	35

Table 6.15 Properties of Streams at average temperature

Property	Product Mixture	Water
Specific Heat, C_p (kJ/kg-K)	3.360	4.224
Density, ρ (kg/m ³)	785	1003.567
Thermal Conductivity, k (W/m-K)	0.5245	0.618239
Viscosity, μ (kg/m-s)	0.00095	0.000797232

From heat balance the mass flow rate of cold fluid was found to be = 0.68605kg/s

Table 6.15 gives the properties of the product mixture and water at average temperature

Table 6.16 Pipe Dimensions

Triangular Pitch, P_t	0.02m
BWG	16
Outer diameter of inner pipe, d_o	0.016m
Inner diameter of inner pipe, d_i	0.014m
Standard Length of Pipe, L_r	3.5 m

Table 6.16 shows the standard pipe dimensions

Logarithmic Mean Temperature Difference Calculations

$$LMTD = \frac{(Thi - Tco) - (Tho - Tci)}{\ln \frac{(Thi - Tco)}{(Tho - Tci)}}$$

Assumptions:

1. 1-2 pass STHE
2. Product gases flow on the shell side and water on the tube side

Table 6.17 LMTD Calculations

$R = (T1 - T2) / (t2 - t1)$	0.8
$S = (t2 - t1) / (T1 - t1)$	0.6
Correction Factor, F_t	0.6
Log mean temperature, ΔT_{LMTD} ($^{\circ}C$)	34.76
Corrected log mean temperature, ΔT_{LMTD} ($^{\circ}C$)	20.57

Table 6.4 shows the calculations for logarithmic mean temperature

Tube side and shell side heat transfer coefficient calculations

Table 6.18 General Specifications

Assume heat transfer Coefficient	U_o	567.83
Heat transfer Area	$A = Q / (U_o \times \Delta T_{LMTD})$	$12.2766 W/m^2 \cdot C^0$
Number of tubes	$n = A / \pi d_o L_r$	65.40
Number of tubes (TEMA P or S)		67
Shell diameter	D_s	1.372 m
Baffle spacing	$D_s/5$	0.27444 m

Table 6.18 gives the general specification in a condenser

Table 6.19 Tube side heat transfer properties

Flow area	$A_t = N(\pi/4) d_i^2$	0.0004 m ²
Mass velocity	$G = m / A_t$	2228.16 kg/ m ² -s
Reynolds number	$N_{Re} = (d_i \times G) / \mu$	43379.55
Prandtl number	$N_{Pr} = (C_p \times \mu) / k$	4.833
Nusselt number	$N_{Nu} = 0.023 \times Re^{0.8} \times Pr^{0.33}$	198.3
Inside heat transfer coefficient	$h_t = N_{Nu} \times k / d_i$	8799.133 W/m ² -C ⁰

Table 6.4 shows the calculations for inner heat transfer coefficient

Table 6.20 Shell side heat transfer properties

Average temperature	$T_{c_{avg}}$	35 C ⁰
Vapour temperature	$T_{h_{avg}}$	70 C ⁰
ΔT_f	$T_{h_{avg}} - T_{c_{avg}}$	35 C ⁰
Bundle diameter	$D_b = d_o \times [N_t / k]^{1/3}$	0.226 m
N_{tf}	$N_{tf} = 2/3 \times [D_b / P_t]$	28.31844
Shell side heat transfer coefficient		4508.41 W/m ² -C ⁰

Table 6.4 shows the calculations for shell side heat transfer coefficient

Table 6.21 Overall heat transfer coefficient

Dirt factor	R_D	0.0008805 m ² -C ⁰ /W
1/U	$(1/h_s) + (1/h_t) + R_D$	0.0012159 m ² -C ⁰ /W
Overall heat transfer coefficient	U	822.39868 W/m ² -C ⁰

Table 6.4 shows the calculations for overall heat transfer coefficient

Overall heat transfer coefficient is greater than assumed heat transfer coefficient. Design for condenser is accepted as a result.

Pressure drop calculations
Table 6.22 Tube side pressure drop calculations

Friction factor	j_F	0.0024
Number of passes	N_p	2
Pressure drop	$\Delta P_t = N_p [8 j_F (L/d_i) + 2.5] U_t^2 \rho / 2$	0.1328 kPa

Table 6.22 shows the pressure drop calculation across the condenser

Mechanical Design

$$\text{Wall thickness, } t = \frac{P \times D}{200 \times f \times J - P} + C$$

Where,

t = thickness in mm

P = operating pressure in kgf/cm² (1 atm = 1.0332 kgf/cm²)

D = diameter of column in mm (1372 mm)

f = allowable stress (13)

J = joint efficiency (0.85)

C = corrosion allowance (min 5 mm)

$$t = \frac{1 \times 1.032 \times 1372}{(200 \times 13 \times 0.85) - 1 \times 1.0332} + 5 = 5.641 \text{ mm}$$

The thickness of the shell is 5.641 mm

The net profit generated by a chemical plant is often a measure of its credibility. In economics and cost estimation, we study the net profit obtained from a plant and the various component costs involved in it. The rate of return and the payback period was also estimated.

7.1 Equipment costs

Table 7.1 List of equipments and costs

S.No	Equipment	Quantity	Cost (in INR)
1	Reactor	1	25287354.6
2	Heat exchanger	2	6453333.334
3	Separator	1	1352569.817
4	Distillation column	2	30714285.72
5	Condenser	2	1430742.858
6	Reboiler	2	5460714.286
	TOTAL		70699000.62

Total equipment costs (E) = 70699000.62 INR

Table 7.1 Includes the list of equipments and its costs for the production of isopropyl alcohol

Table 7.2 Factors contributing to direct costs

Additional expenses on equipment	% of equipment cost	Cost (in INR)
Equipment Installation	25	17674750.15
Transportation and Local Tax	5	3534950.031
Instrumentation	15	10604850.09
Packing and Installation	10	7069900.062

Electrical Assembly	10	7069900.062
Building (including services)	40	28279600.25
Cost of Land	30	21209700.18
Services and Maintenance	7	4948930.043
TOTAL		100392580.9

Total direct costs = 100392580.9 INR

Table 7.2 shows the factors contributing to direct costs for the production of isopropyl alcohol

7.2 Indirect costs

Table 7.3 Indirect costs

Services	% of equipment cost	Cost (in INR)
Engineering expense and supervision	20	14139800.12
Construction expenses	20	14139800.12
TOTAL		28279600.25

Table 7.3 shows the indirect costs for the production of isopropyl alcohol

Fixed Capital Investment = Direct costs + Indirect costs
 = 100392580.9 + 28279600.25 = 128672181.1 INR

7.3 Factors Contributing to FCI

Table 7.4 Factors contributing to FCI

Names	% FCI	Cost (in INR)
Contractor fees	5	6433609.056
Contingencies	10	12867218.11
TOTAL		19300827.17

Table 7.4 shows the factors which contribute to FCI for the production of isopropyl alcohol

$$\text{Total FCI} = 128672181.1 + 19300827.17$$

$$= 147973008.3 \text{ INR}$$

$$\text{Total Capital Investment} = \text{FCI} + \text{Working Capital Investment (15\% of TCI)}$$

$$0.85 \times \text{TCI} = 147973008.3 \text{ INR}$$

$$\text{Total Capital Investment} = 174085892.1 \text{ INR}$$

$$\text{Working Capital Investment} = 26112883.82 \text{ INR}$$

7.4 Total Product Costs

$$\text{Total product cost} = \text{Manufacturing cost} + \text{General expenses}$$

Where,

$$\text{Manufacturing cost} = \text{Direct production costs} + \text{Fixed Charges}$$

Table 7.5 Factors contributing to fixed charges

Items	% of FCI	Cost (in INR)
Depreciation	10	14797300.83
Local taxes	3	4439190.249
Insurance	1	1479730.083
Rent	10	14797300.83
TOTAL		35513521.99

Table 7.5 shows the factors which contribute to fixed charges for the production of isopropyl alcohol

Table 7.6 Factors contributing to direct production costs

Items	% of TPC	Cost (in INR)
Raw Material	30	0.3X
Operating Labour	15	0.15X
Direct Supervisory and electrical labour	3	0.03X
Utilities	15	0.15X
R&M	5	30086499.73
Operating Supply	10	3008649.973
Labour Charges	15	451297.4959
Patents	5	0.05X
Plant Overhead Cost	10	0.1X
TOTAL		0.78X + 33546477.19

Table 7.6 shows the factors which contribute to direct production costs for the production of Isopropyl alcohol

Where Total production cost is assumed as X

7.5 General Expenses

Table 7.7 General expenses

Items	% of TPC	Cost (in INR)
Administrative Cost	4	0.04X
Distribution and Selling Cost	10	0.1X
R &D	5	0.05X
TOTAL		0.19X

Table 7.5 includes the general expenses for the production of isopropyl alcohol

Manufacturing Costs = Fixed Charges + Direct Production Costs

$$= 35513521.99 + 0.78X + 33546477.19$$

$$= 69059999.18 + 0.78X$$

Total Production Costs = Manufacturing cost + General expenses

$$X = 2301999973 \text{ INR}$$

Therefore, Total production costs = 1516549852 INR per year

7.6 Estimation of Total Income

Selling price of IPA = Rs. 129 per kg

Annual working days = 365

Production rate = 18250000 kg per year

$$= 50000 \text{ kg per day}$$

Total income = (Selling price of IPA x Production rate (in days) x Annual working days)

$$= (129 \times 50000 \times 365) = 2354250000 \text{ INR}$$

Gross Income = Total income – Total production costs

$$= 2354250000 - 2301999973 = 52250027 \text{ INR}$$

Tax rate = 30 % of Gross Income

Therefore, tax paid = 15675008.21 per year

Net profit = Gross income – Tax paid

$$= 52250027 - 15675008.21 = 36575019.16 \text{ INR}$$

Rate of Return = (Net Profit/ Total Capital Investment) x100

$$= 36575019.16/174085892.1 = 21.01 \%$$

Payback period = (Total Capital Investment/Net Profit)

$$= 174085892.1/36575019.16$$

$$= 4.76 \text{ years}$$

The location of plant is a very important and crucial step once process is selected. Many factors must be considered while selecting suitable site mainly the raw materials, market, infra-structure, water resources and impact on an adjacent ecologic systems. Also the process selected plays a major role in the location of the plant.

8.1 Plant Location

The important criteria are affecting site selection:

- Availability of suitable land
- Raw material supply
- Proximity to sea
- Labor availability
- Proximity to infrastructure facilities like road, rail, and ports etc
- Ease of effluent disposal
- Availability of marketing area
- The impact on the adjacent ecological systems
- Availability of utilities
- Climate

8.1.1 Raw materials

The process has been selected as Tokoyama process which uses ammonia to produce nitric acid. Therefore the availability and price of these raw materials is important in the site selection. It is preferred that the plant is located in close proximity where propylene is easily available.

8.1.2 Market availability

Isopropyl alcohol when produced in bulk quantities the cost of the product per ton is relatively low and the cost of transport. To get a significant fraction of sales price, the plants should be located close primary market.

8.1.3 Transport

The material transport is one of the effective principal factors of site location. In practice the plant should be located in a place where these two major forms of transport are available: road and water

way. Road transport is being mainly used for local distribution from warehouse. Rail transport is a type of road transport and will be cheaper for long distance transport of bulk chemicals. Water way used for international transport of raw materials and products.

8.1.4 Availability of Utilities

Plant utilities are the important parameter for any plant. The plant should be located where all the utilities are available in enough quantities. Following are the important utilities for nitric acid plant are

- Steam
- Cooling water
- Electricity
- Refrigeration

8.1.5 Climate

The dry and sunny condition that is present throughout the year is extremely suitable for a process plant because loss of heat by cooling of process due to rain is avoided. This also saves energy and makes it possible to obtain consistent product quality.

8.1.6 Effluent disposal

All industrial processes produce waste product, the waste has to be treated and disposed properly without causing any harm to environment.

8.2 Plant Layout

Preparing a suitable plant layout for the selected site is the immediate step once the plant location is decided. The economic construction and efficient operation of process unit will depend on how well the plant and equipment specified on the process flow sheet is laid out.

The principle factors of plant layout considered are,

1. Economic consideration: installation and operating costs
2. The process requirement

3. Ease of plant operation
4. Maintenance
5. Safety
6. Future expansion

A reference plant layout is shown in figure 8.1

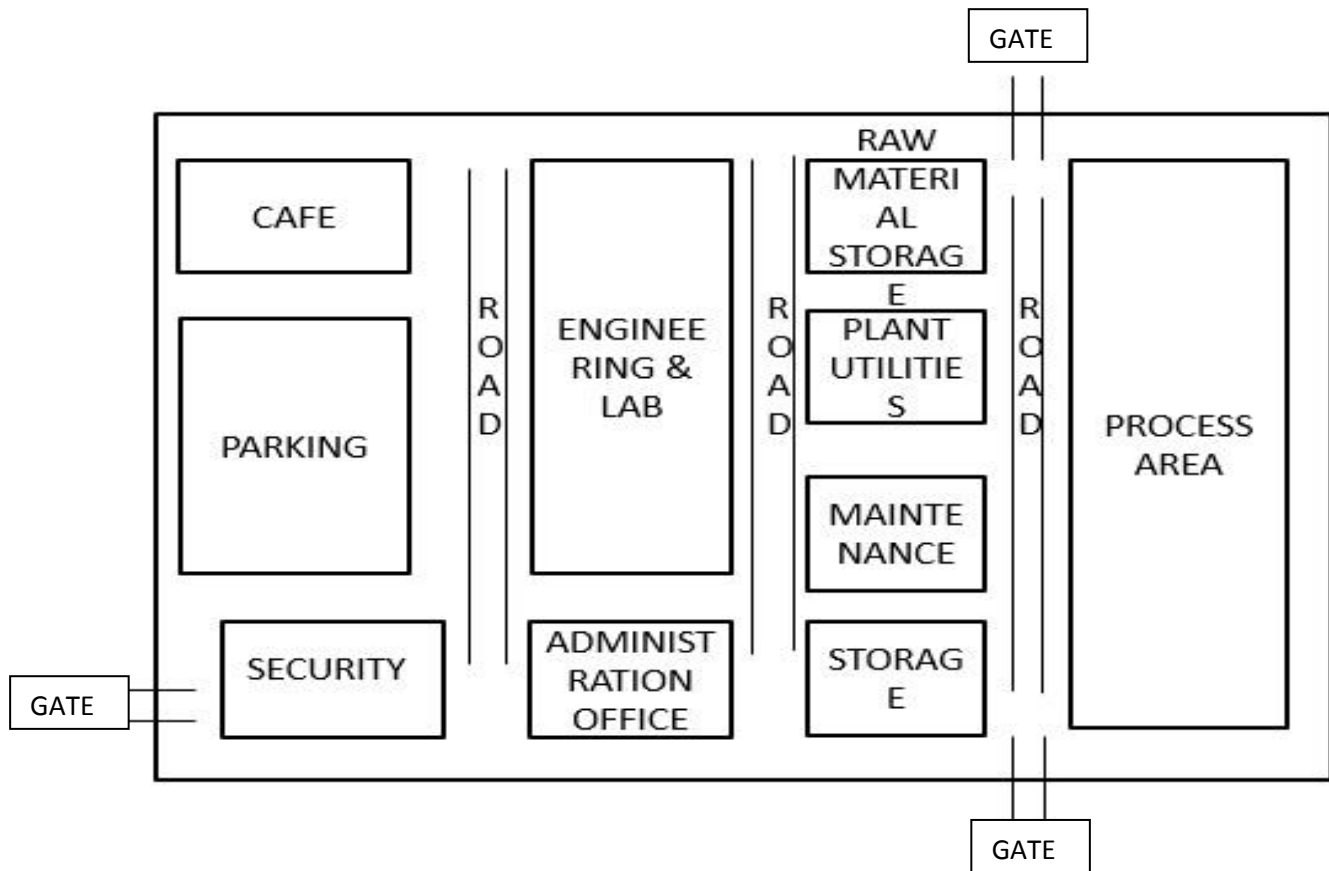


Figure 8.1 Reference plant layout for the production of Isopropyl alcohol 50 tons/day

8.3 Site Selection

Figure 8.2 shows the chosen location, Yerawada in Pune for our process plant.

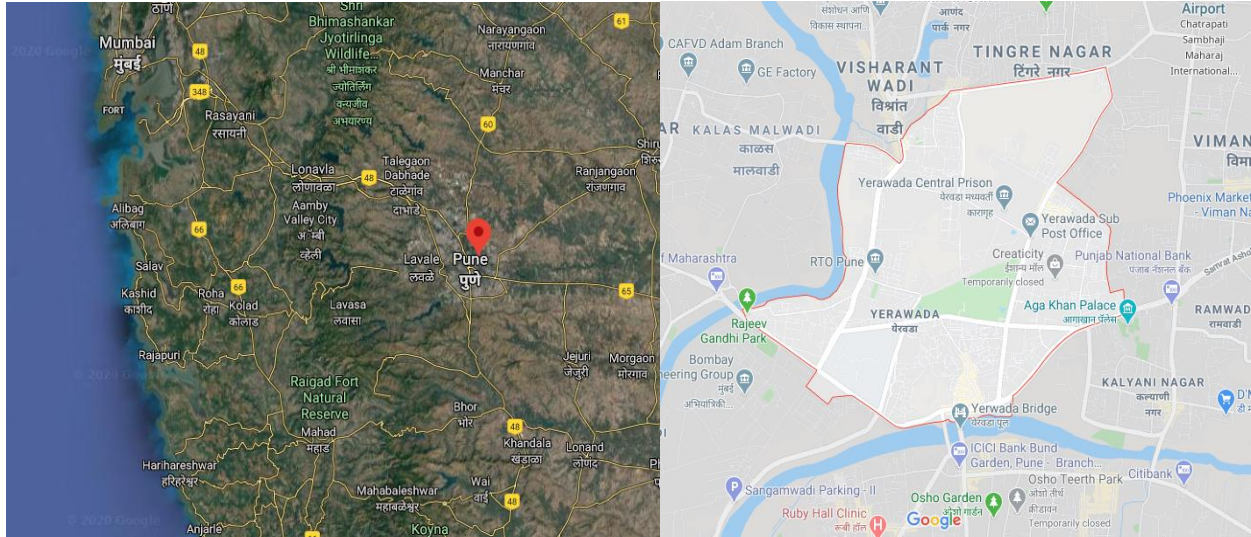


Figure 8.2 Referential plant location selected for the production of Isopropyl alcohol 50 /tons per day

A P&I diagram shows information on piping, fittings, equipment, instrumentation, and process plant in a representative and sequential arrangement on the basis of product flow paths. Installation of piping and instrumentation in process flow path plays a very important role in optimization of controlled process flow. Considering the above requirement the control systems has to be introduced to provide safe operation and controlled output flow.

The PID should include,

- Instrumentation and designations.
- Mechanical equipment with names and numbers.
- All valves and their identifications
- Process piping, sizes and identification.
- Miscellaneous-vents, drains, special fittings, sampling lines, reducers, and increasers.
- Flow direction.
- Computer control system input interconnections references.

9.1 Equipments of P&ID

Equipment of PID comprised of hardware like compressors, conveyors, motors, turbines, vacuums and other mechanical devices.

Piping: A pipe is a tube that transports fluid substances. Piping can be made of various materials including metal and plastic. The piping group is made up of one-to-many pipes multiline pipes, separators and other type of piping devices.

Heat exchangers: It is a device that is designed to efficiently transfer heat from different areas or medium this includes boilers, condensers, and other heat exchangers.

Pumps: It is a device that uses suction or pressure to rise, compress or move fluids in and out of other objects. This section is comprised of both pumps and fans.

Instruments: An instrument is a device that measures and sometime controls flow, temperature, angle or pressure. The instruments group houses indicators, controllers, recording, transmitters and elements.

Valves: It regulates, directs or controls the flow of a fluid by opening, closing or partially obstructing passage ways in a piping system. This category includes rotameter, orifice and other types of valves.

9.2 Piping and Instrumentation Diagram of the Plant

Figure 9.1 depicts the P&I diagram of the current Isopropyl Alcohol plant

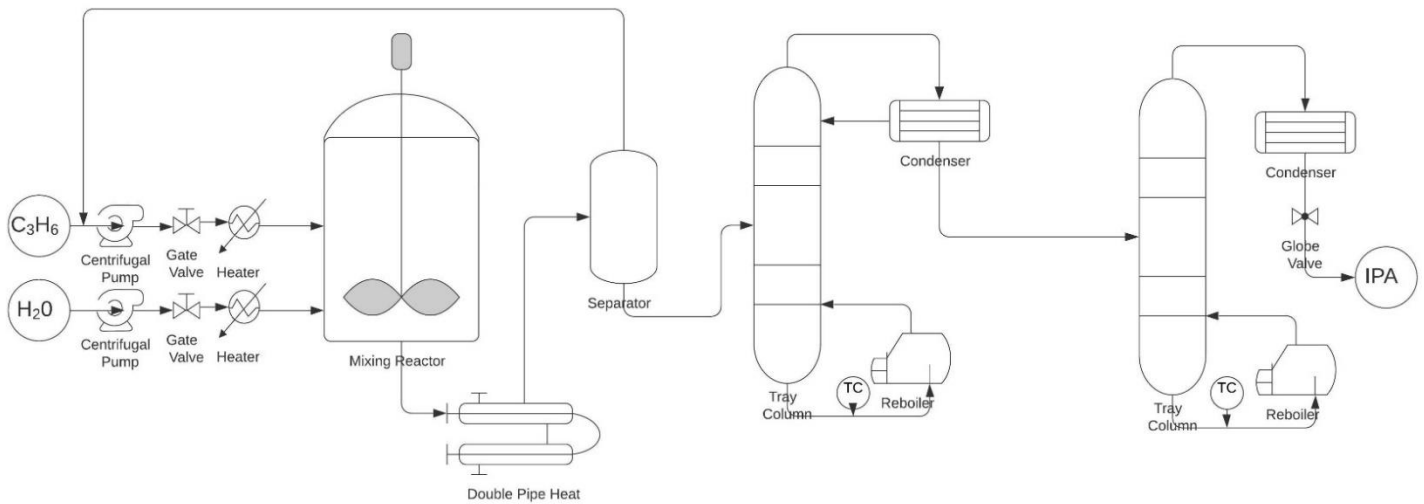


Fig 9.1 P&ID of the plant for production of Isopropyl alcohol

This chapter discusses about some safety measure that should be taken when handling isopropyl alcohol and isopropyl products, as a preventative measure.

- **CAS Registry No:** 67-63-0
- **Synonyms :** 1-methylethanol, 1-methylethyl alcohol, 2-hydroxypropane, dimethyl carbinol, ethyl carbinol, hydroxypropane , IPA, i-propanol, isoethylcarbinol propan-2-ol, sec-propanol
- **Formula :** C₃H₈O
- **Use:** Disinfectant Solvent, Laboratory chemicals

10.1 Hazard Identification

Flammable liquids: Category 2

Highly flammable liquid and vapor

Serious eye damage/eye irritation Category 2A

Causes serious eye irritation Specific target organ toxicity Category 3

May cause respiratory irritation

10.2 First aid measures

- **Inhalation:** Remove the victim into fresh air. Respiratory problems: consult a doctor/medical service.
- **Skin contact:** Rinse with water. Do not apply (chemical) neutralizing agents without medical advice. Soap may be used. Take victim to a doctor if irritation persists.
- **Eye contact:** Rinse immediately with plenty of water. Remove contact lenses, if present and easy to do. Continue rinsing. Do not apply (chemical) neutralizing agents without medical advice. Take victim to an ophthalmologist if irritation persists.
- **Ingestion:** Rinse mouth with water. Do not apply (chemical) neutralizing agents without medical advice. Immediately after ingestion: give lots of water to drink. Do not induce vomiting. Call Poison Information Centre (www.big.be/antigif.htm). Consult a doctor/medical service if you feel unwell. Ingestion of large quantities: immediately to hospital. Take the container/vomit to the doctor/hospital.

10.3 Handling and Storage

- **Additional hazards when processed:** May form explosive peroxides.
- **Precautions for safe handling:** Use spark/explosion proof appliances and lighting system. Take precautions against electrostatic charges. Keep away from naked flames/heat. Keep away from ignition sources/sparks. Measure the concentration in the air regularly. Work under local exhaust/ventilation. Comply with the legal requirements. Remove contaminated clothing immediately. Clean contaminated clothing. Handle unclean empty containers as full ones. Thoroughly clean/dry the installation before use. Do not discharge the waste into the drain. Do not use compressed air for pumping over. Keep container tightly closed.
- **Hygiene measures:** Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Wash contaminated clothing before reuse.
- **Heat-ignition:** Keep substance away from heat sources and ignition sources.
- **Prohibitions on mixed storage:** Keep substance away from: oxidizing agents. Strong acids. (Strong) bases. Amines. Halogens.
- **Storage area:** Store in a cool area. Store in a dry area. Ventilation at floor level. Fireproof storeroom. Provide for an automatic sprinkler system. Provide for a tub to collect spills. Provide the tank with earthing. May be stored under nitrogen. Meet the legal requirements.
- **Special rules on packaging:** Closing with pressure relief valve. Dry. Clean. Correctly labeled. Meet the legal requirements. Secure fragile packaging's in solid containers.
- **Packaging materials:** stainless steel. Monel steel. Carbon steel. Copper. Nickel. Bronze. Glass. Teflon. Polyethylene. Polypropylene. Zinc. Material to avoid: steel with rubber inner lining. Aluminum.

10.4 Accidental release Measures

General Measures: Clean up any spills as soon as possible, using an absorbent material to collect it.

For Non-Emergency Personnel

- Protective equipment: Gloves. Protective goggles. Protective clothing. Large spills/in enclosed spaces: compressed air apparatus.
- Emergency procedures: Keep upwind. Mark the danger area. Consider evacuation. Seal off low-lying areas. Close doors and windows of adjacent premises. Stop engines and no smoking. No naked flames or sparks. Spark- and explosion-proof appliances and lighting equipment. Keep containers closed. Wash contaminated clothes.

For Emergency Responder's

- Protective equipment: Equip cleanup crew with proper protection. Do not breathe gas, fumes, vapor or spray.
- Emergency procedures: Stop leak if safe to do so. Ventilate area. If a major spill occurs, all personnel should be immediately evacuated and the area ventilated.

References

1. Kirk-othmer encyclopedia 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
5. Isopropyl Alcohol by Direct Hydration of Propylene by Yasuharu Onoue, Yukio Mizutani, Sumio Akiyama, Yusuke Izumi and Hirofumi Ihara.
6. [https://doi.org/10.1016/0009-2509\(84\)80041-X](https://doi.org/10.1016/0009-2509(84)80041-X)
7. <https://www.britannica.com/science/isopropyl-alcohol>
8. <https://www.imarcgroup.com/global-isopropyl-alcohol-market>
9. <https://indianpetrochem.com/report/isopropylalcoholreport>
10. <https://www.marketresearchfuture.com/reports/isopropyl-alcohol-market-1078>
11. <http://www.inchem.org/documents/pims/chemical/pim290.htm>
12. https://neutrium.net/fluid_flow/estimating-the-viscosity-of-mixtures/
13. <https://webbook.nist.gov/cgi/fluid.cgi?TUnit=C&PUnit=atm&DUnit=kg%2Fm3&HUnit=kJ%2Fkg&WUnit=m%2Fs&VisUnit=cP&STUnit=N%2Fm&Type=IsoTherm&RefState=DEF&Action=Page&ID=C115071>
14. <https://pubs.acs.org/doi/10.1021/je00035a019>
15. <https://www.ncbi.nlm.nih.gov/pmc/articles/PMC5094801/>
16. <https://webbook.nist.gov/cgi/cbook.cgi?ID=C67630&Mask=2>
17. Richard M. Felder and Ronald W. Rousseau, Elementary Principles of Chemical Processes, John Wiley & Sons, 3rd Edition, 2005. Dryden's outlines of chemical technology.
18. Levenspiel, O., Chemical Reaction Engineering, 3rd Edition, John Wiley & Sons, 2001.
19. Perry's Chemical Engineers Handbook.
20. Smith, J.M. and Vanness, H.C., Introduction to Chemical Engineering Thermodynamics, 5th Edition, McGraw Hill, New York 1996.
21. Treybal, R.E., Mass Transfer Operations, 3rd Edition, McGraw Hill, 1981.
22. Dutta, B.K., Principles of Mass Transfer and Separation Processes, 1st Edition, PHI, 2006.
23. McCabe, Unit Operations of Chemical Engineering, McGraw Hill, NY, 5th Edition, 2000.

24. Kern, D. Q., Process Heat Transfer, McGraw Hill, NY, 1965.
25. Joshi, M.V., Process Equipment Design, Macmillan India, 1991.
26. Peters and Timmerhaus, Plant Design and Economics for Chemical Engineers, McGraw Hill, 5th edition, 2003.