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Research Article

Simulation and Performance Assessment of a Pure Acetone Production Facility via Isopropanol Dehydrogenation in a Heterogeneous Catalytic Reactor.

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Abstract: Nowadays, considering the country's extensive need for acetone as a strategic product, innovative processes for its production can be explored. Up to 75% of the formulation and production of chemical and healthcare products are influenced by the presence of this valuable product in their structure. Among the older processes for acetone production, direct hydroperoxide conversion of cumene according to the Wacker-Hoechst method and direct acetone production from phenol according to the Hock method can be mentioned. In this article, an acetone production process using hydrogenation of inexpensive 2-propanol feedstock is simulated with the help of Aspen HYSYS and Aspen Plus software, utilizing first-order kinetics and industrial data. Subsequently, necessary optimizations were made to prevent water wastage and achieve 98-99% pure acetone production by reclaiming two additional water streams and part of the unused reaction feed. The acetone production process, based on hydrogenation, has led to increased purity in the production unit compared to standard and old methods, along with a 32% reduction in energy consumption due to the utilization of a novel process. This method lacks explosion risks associated with high pressure and temperature in the reactor, typically accompanied by oxygenated water in conventional acetone production methods.

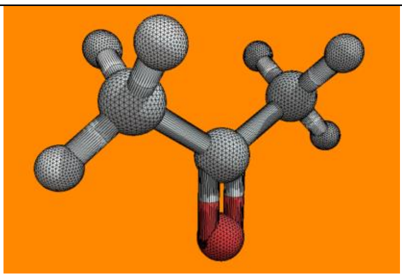
Keywords: Simulation, Acetone, Isopropyl alcohol, Catalytic reactor, Aspen.

1. Introduction

Acetone, the simplest ketone found in nature with the chemical formula C_3H_6O, is a highly volatile organic compound with a low boiling point, readily evaporating in air and soluble in water. This valuable substance was first discovered by the scientist James Dewar [1]. In industry, acetone is referred to by various names such as dimethyl ketone, propanone, dimethyl formaldehyde, and dimethyl carbonyl. Acetone serves as a solvent for cellulose acetate and nitrocellulose, as well as a ketone for hexylene glycol (-2-methyl-4,2-pentanediol) and a carrier for isopropyl alcohol [2, 3]. Additionally, this valuable solvent is used as a raw material for synthesizing a wide range of ketones, methyl methacrylate, phenols, alcohols, and methyl isobutyl ketones. The properties and chemical structure of acetone are outlined in Table 1.

Table 1. Chemical Structure and Properties of Acetone

Three Dimension of Acetone



Property	Value	Dimension	Reference
Molecular Weight	58.08	[gr/mole]	[4]
Physical state	Liquid	-----------	[2]
Color	Colorless and transparent	-----------	[1]
Flash point	-17.8	Celsius degrees	[5]
Boiling point at 760 mmHg	560	Celsius degrees	[5]
Freezing Point	-93.9	Celsius degrees	[1]
Vapor Density/Air Density	2	-----------	[2]
Vapor Pressure at 20 Celsius degree	24.2	[Kpa]	[3]
Viscosity at 15 Celsius degree	0.3371	[Cp]	[4]
Solubility at water	Mixable for all values	-----------	[4]
Specific gravity at 25 Celsius degree	0.7860	-----------	[1]
Commercial grade purity	97-99	[%]	[2]
Weight percentage of water in Acetone	3:0.5	[%]	[4]
Maximum Acidity Factor	0.002	-----------	[5]
Maximum Alkaline Factor	58.08	-----------	[5]

Until the early stages of World War I, acetone was produced by distilling calcium acetateand then, due to the neutralization of sulfuric acid with the lime produced, industrial units began to use it. During World War I, the acetone production process was developed by bacterial fermentation by scientist Chaim Weizmann, producing acetone, butanol, and ethanol [6]. Over time, due to its low efficiency compared to other organic waste of this process, the production of this substance was forgotten. In the past, Weizmann and Hammline proposed a method for industrial-scale acetone production [7]. In 1974, 65% of the total acetone production in the world was from the cumene hydroperoxide method. However, today, new methods are proposed to compensate for the shortcomings and risks of this method for acetone production. Acetone production by the hydrogenation of isopropyl alcohol feedstock began indirectly in the early 1920s [8]. Among the industrial production methods, the two direct production methods of acetone by propylene oxidation and acetone production from isopropyl alcohol feedstock by hydrogenation have the most industrial applications. Currently, three different processes are licensed for acetone production: the cumene process, thepropylene oxidation process, and the isopropyl alcohol process. Table 2 compares the advantages and disadvantages of these three acetone production methods.

Table 2. Comparison of Industrial Acetone Production Methods: Advantages and Disadvantages

	Process Name	Advantages	Disadvantages
1.	Cumene Process	The most common method	High energy consumption Low product quality High Risk Explosion
2.	Propylene Oxidation	Very safe process Less hazardous	Low production rate Not cost effective
3.	Hydrogenation	Hight Purity Low explosion risk High conversion Efficient process	--------

2. Materials and Methods

In several countries, acetone is produced by the Cumene Hydroperoxide process under a license agreement with Shell and Du Pont. However, the traditional process was not without problems like high reactor pressure, explosion, and fire hazards attributed to the production of oxygenated water, which challenged the licensed chemical companies to look for better chemical processes to produce quality acetone [9]. In this work, aspiration simulation of acetone production was carried out and the software used included Aspen HYSYS and Aspen Plus based on actual PFDs and PIDs collected from the industry. The simulation was oriented on minimizing energy utilization to achieve the desired conditions and avoiding water losses in the absorber tower. Particularly, two water streams were re-utilized within the process, namely the first one coming from the isopropyl alcohol separator tower and the second one belonging to the recycle stream containing isopropyl alcohol and lighter water was directed as feed to the absorber tower and the catalytic reactor.

In the above simulations, important optimizations that were affected sought to produce acetone with a maximum purity of 99. 83%. These optimizations included; deciding on the right number of trays in the acetone separator tower, improving the process water recovery, deciding on the right operating pressure of the separator towers and investigating the effects of a heat exchanger before the tower. The process equipment was carefully evaluated and redesigned for these changes according to the simulation result as follows: These changes make it possible to obtain high purity of acetone up to 99%. 75% is free from impurities and better in quality than the previous conventional methods. In addition, the simulation sought to solve for forming an azeotrope in the isopropyl alcohol separator tower where some of the water will remain within the isopropyl alcohol and cannot be separated easily. On the tower level, after researching the azeotrope formation region, another possibility was analyzed to boost the overall effectiveness of the process – the recycling of the above-mentioned stream with fresh feed.

2.1. Process Description

According to the hydrogenation method for producing acetone from isopropyl alcohol, the process requires a gas-phase catalytic reactor, an absorber tower, an acetone separator tower, an isopropyl alcohol separator tower, a heat exchanger, cooling towers, centrifugal pumps, mixers, and other devices and equipment embedded in the overall process diagram which is shown in Figure 1.

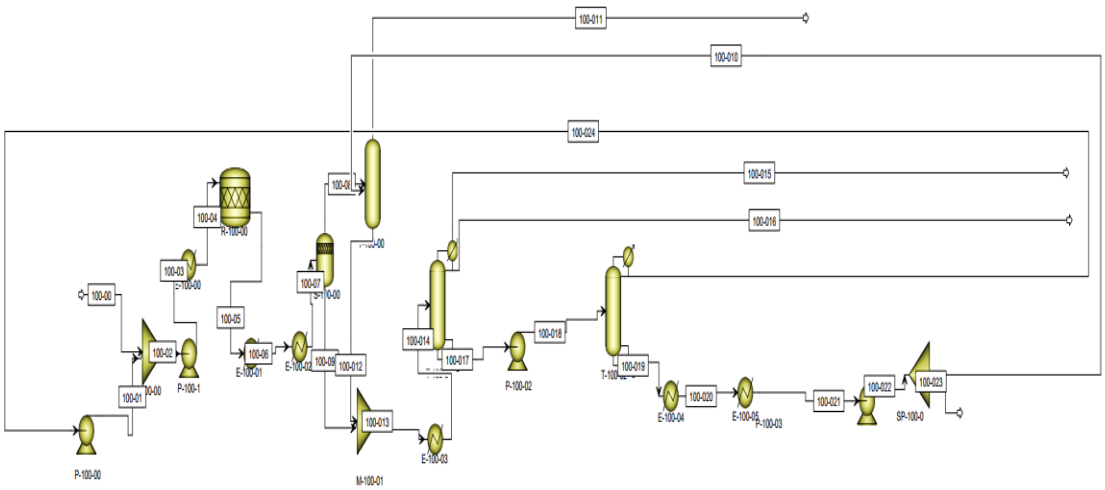


Figure 1. Process Flow Diagram for Acetone Production from Isopropanol via Hydrogenation

2.1.1 Feed Preparation

The feed to the process, as per Table 3, after being mixed with the recycle stream, enters the centrifugal pump with a 75% capacity, according to Figure 1. This feed is then introduced into the reactor by this pump to achieve optimal operating conditions, with temperatures ranging from 25 to 35 degrees Celsius and pressures ranging from 120 to 140 kilopascals.

Table 3. Feed Specifications

Parameter	Details	Value	Dimension	Reference
Feed Composition	IPA[1]	65	[%]	[3]
	Water	35	[%]	[3]
Feed Molar Flow	--------	136.4	[kmole/hr]	[5]
Feed Pressure	--------	120	[Kpa]	[7]
Feed Temperature	--------	28	[Celsius degrees]	[7]

2.1.2 Kinetic of reaction

The conversion reaction of isopropyl alcohol to acetone in the catalytic reactor is highly exothermic, occurring according to the following reaction. The extent of conversion of isopropyl alcohol to acetone in the catalytic reactor, is logarithmically related to the reaction rate constant according to equations 1,2 and 3. According to eqaution1, activation energy is 72.38 megajoule per kilomole. In this relationship, T represents the temperature of the outlet stream of the catalytic hydrogenation reactor in Kelvin, and P represents the pressure of the outlet stream of the catalytic hydrogenation reactor in atmospheres. In these equations, the parameter X represents the conversion rate in percentage, in the catalytic reactor using the hydrogenation method

$$-r_{IPA} = K_0 \exp[\frac{-Ea}{RT}]C_{IPA} \qquad \text{Eq (1)}$$

$$LogKp = -\frac{2758}{T} + 1.510 LogT + 1.759 \qquad \text{Eq (2)}$$

$$X = (\frac{Kp}{p + Kp})^{0.5} \qquad \text{Eq (3)}$$

[1] Isopropanol Alcohol

2.1.3 Absorber Column

To ensure complete separation of hydrogen in the vapor phase, a two-phase separator, as per the license, has been installed before entering the absorber tower. The solvent used in this tower is water, due to its availability and low industrial cost [10, 11]. The incoming water stream to the highest tray of the tower consists of a combination of pure water recirculated from the water separator tower and fresh water entering the absorption unit. Another inlet stream to the hydrogen absorption tower is the vapor stream exiting the flash drum, which is introduced into the tower from the lowest tray for mass transfer to achieve maximum hydrogen separation. The specifications of the hydrogen absorption tower are provided in Table 4.

Table 4. Absorber Column Specifications

Parameter	Value	Dimension	Reference
Top Column Temperature	15	[Celsius degrees]	[10]
Bottom Column Temperature	27	[Celsius degrees]	[10-13]
Top Column Pressure	3.5	[atm]	[12]
Bottom Column Pressure	5	[atm]	[14]
Feed Stage	12,1	--------	[15]

2.1.4 Water Separation Column

In this tower, due to the formation of an azeotrope between isopropyl alcohol and water in the temperature range of 75-90 degrees Celsius, a portion of isopropyl alcohol always exits the tower along with water as it does not participate in the reaction [12-14]. After examining and plotting the azeotrope formation diagrams in this article, this stream is returned to the initial mixer for reuse. After mixing with fresh feed, it serves as the feed stream to the acetone-producing reactor in the process. Figure 2 illustrates the formation of an azeotrope in the isopropyl alcohol and water separator tower using the NRTL thermodynamic model due to the polar nature of the compounds [6, 15].

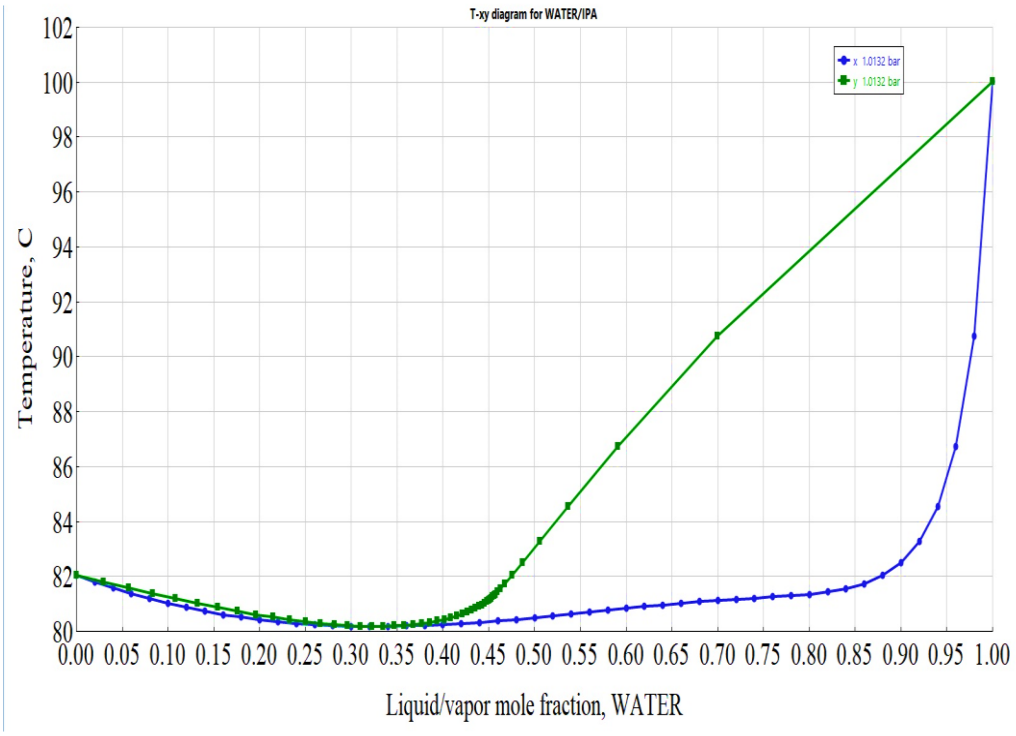


Figure 2. T-xy diagram for IPA/WATER

3. Results and decision

3.1 Absorber Column Performance Analyses

The validation of the effect of density distribution plots of vapor and liquid streams on the trays of the hydrogen absorption tower is demonstrated in Figure 3. As depicted, the density of vapor has increased on tray number 10 due to the effective performance of the absorption tower in separating hydrogen from other compounds, indicating an enrichment of hydrogen in the vapor phase [16, 17]. Conversely, on tray number 10, the liquid density has decreased satisfactorily, indicating the presence of remaining heavy components in the heavy stream exiting the tower.

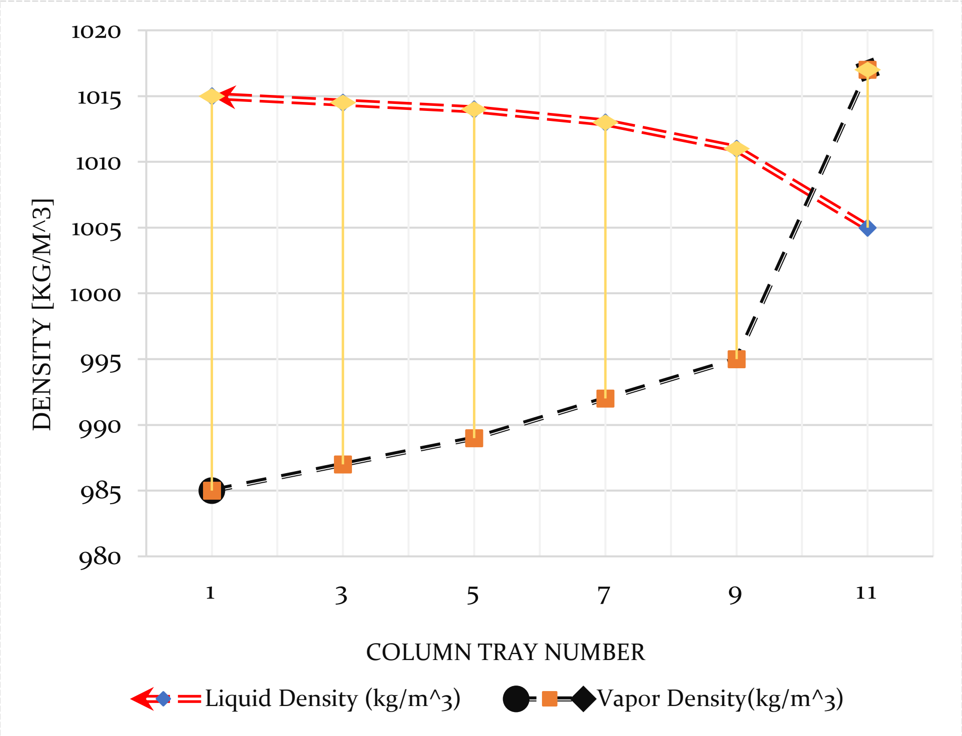


Figure 3. Vapor and Liquid Density Distribution in absorber Column

3.2 Acetone Separation Column

The Temperature, pressure, composition distribution diagrams for the streams on the trays of the acetone distillation tower are illustrated in Figure 4, 5, respectively. As depicted in Figure 4, the optimal temperature range of 25-35 degrees Celsius is chosen for the feed entering the absorption tower to achieve suitable separation in the absorption tower.

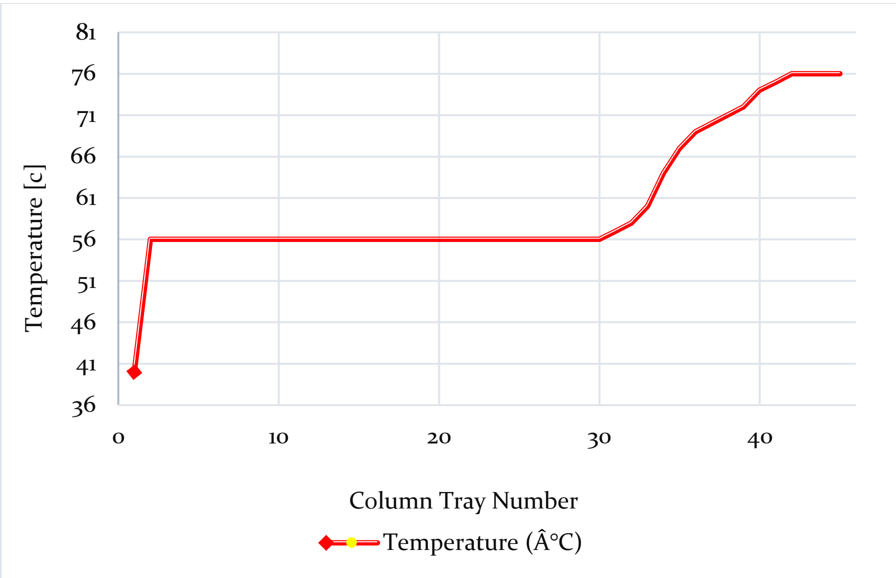


Figure 4. Acetone Column Temperature Distribution

As depicted in Figure 5, the molar fraction of acetone decreases in trays close to the feed tray, indicating the enrichment of the liquid stream exiting with acetone and being free from isopropyl alcohol and water. Additionally, the increasing trend of molar fractions of water and isopropyl alcohol in tray number 35, the feed tray location, signifies the enrichment of the heavy stream exiting from the bottom of the acetone separation tower.

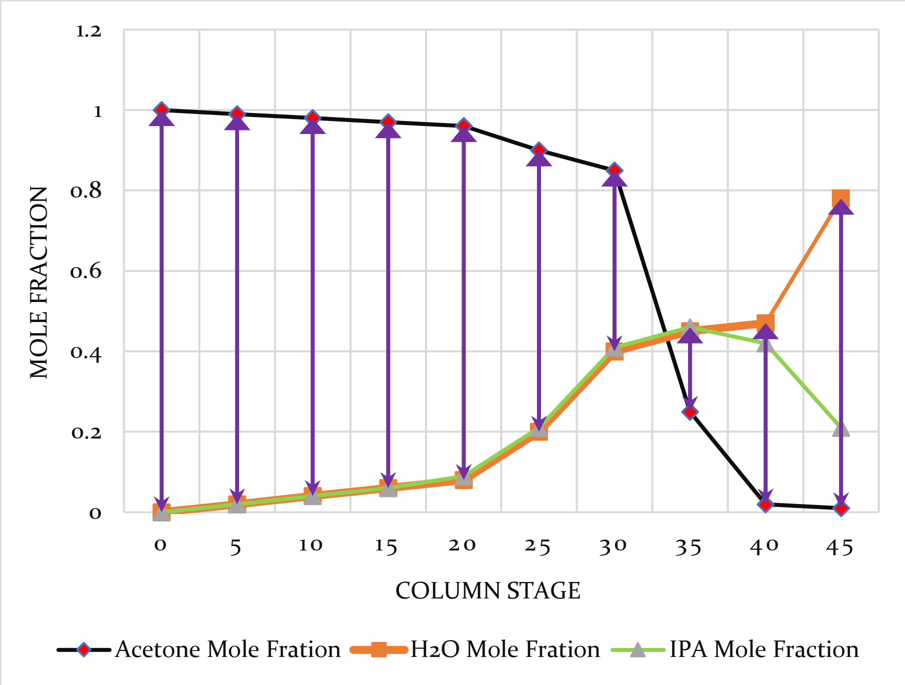


Figure 5. Acetone Column Component Mole Fraction Distribution

As depicted in Figure 6, the novel process for acetone production results in a 32% reduction in energy consumption compared to traditional methods. An important aspect highlighted in this article is the prevention of water wastage, as shown in Figure 7, where a portion of the pure water stream is recycled back into the distillation tower via a high-pressure pump and used as feed for the absorption unit.

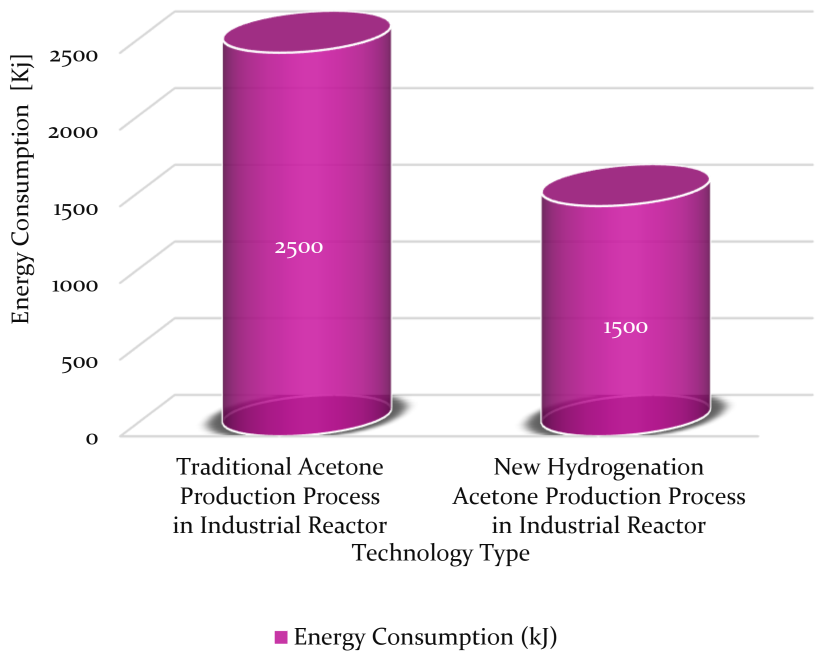


Figure 6. Energy consumption of the acetone production reactor

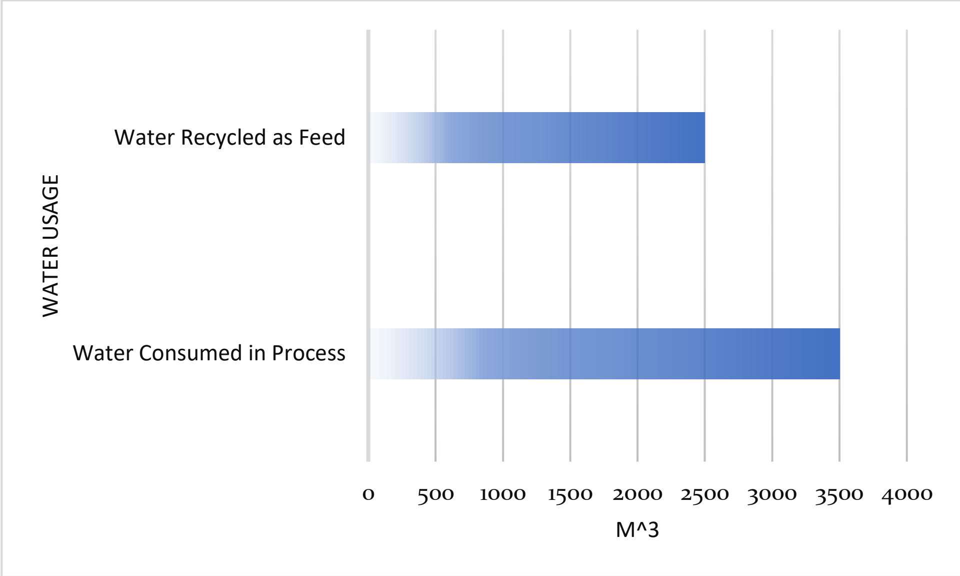


Figure 7. Comparison of Water Consumption and Recycled Water in the Acetone Production Process

4. Conclusions

The production unit of acetone is one of the most important industrial units currently in use in the country, employing old and high-risk methods for acetone production. With the increasing prices of energy carriers and the financial and life risks associated with highly hazardous processes, employing high-tech processes becomes particularly significant. To the best of the author's knowledge, this work is for the first time in Iran, an industrial unit for acetone production from the inexpensive feedstock isopropanol using the hydrogenation method in a catalytic reactor has been simulated The acetone production process from the inexpensive feedstock isopropanol does not have the risks associated with the very high pressures of older processes, resulting in a 32% energy consumption saving compared to older methods, as shown in Figure 13. To produce acetone with a purity of 99.83%, optimization of the operational conditions, such as temperature and pressure of the towers, and using an absorption tower for water were investigated and evaluated. The simulation results using software indicate that due to the formation of an azeotrope in the presence of isopropanol and water in the temperature range of -75 to 90 degrees Celsius, the operational conditions of the water distillation tower are slightly limited. In this simulation, this strength point has been utilized by not returning the feed to the reactor and instead using it for mixing in the absorber with a molar fraction of 65% isopropanol and 35% water.

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