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Research Article

Enhancing of Acetone Purity and Energy Efficiency in the Isopropyl Alcohol (IPA) Dehydrogenation Process Through Design Modifications, Heat Exchanger Integration Simulation, and Reactor Temperature Optimization

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Abstract

Acetone is an essential ingredient in various industries whose demand continues to increase, thus requiring an efficient production method. This study aims to design an acetone production process by dehydrogenating isopropyl alcohol using Aspen HYSYS simulation and Aspen Energy Analyzer energy analysis. The simulation model was developed to enhance the purity of acetone products and improve energy efficiency by optimizing thermodynamic operating conditions. The dehydrogenation process was designed to produce acetone as the main product and hydrogen as a by-product. The basic process was then modified by integrating thermal energy and increasing the reactor operating temperature to improve energy efficiency and product purity. Simulations showed that the process modification resulted in an acetone purity of 99.76%, higher than the base process of 98.46%. In addition, energy savings in the modified process reached 40.89%, higher than the base process of 32.96%, with a reduction in carbon emissions of up to 40.88%. With these results, the modified process proved more efficient than the basic process and aligned with the research objectives.

Keywords: Acetone; isopropyl alcohol dehydrogenation; energy efficiency; product purity; carbon emissions

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1. Introduction

Acetone is one of the leading products in essential organic synthesis with a high global demand, reaching 6 million tons per year and increasing overall demand every year [1,2]. The gap between global acetone production and demand is estimated at 1.7 million tons [3]. Therefore, significantly upgrading acetone into a valuable product is required for a more economical process. As an important raw material in the petrochemical industry, the need for acetone is increasing. However, the availability of petroleum as the leading resource for its production is depleting, posing a challenge in meeting the global demand [4].

Acetone plays an important role in various laboratory and industrial applications. It is used as a chemical intermediate in pharmaceuticals, as well as a vinyl and acrylic resin solvent, and in producing varnishes, alkyd paints, inks, cosmetics, and coatings. In addition, acetone is utilized to manufacture paper coatings, adhesives, and heat seal coatings and as a base material for synthesizing various chemical compounds [5].

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Industrially, acetone can be produced via two main routes, namely cumene hydroperoxide oxidation and isopropyl alcohol (IPA) dehydrogenation [6]. However, cumene-based methods have several disadvantages, such as high production costs, toxic properties, and low efficiency. This encourages the development of alternative methods that are more efficient and environmentally friendly. One of the best alternatives is the IPA-based method. IPA is an economical, easily obtained, cheap, and environmentally friendly raw material [7].

The main advantage of the dehydrogenation process of isopropyl alcohol is that the resulting acetone is free of traces of aromatic compounds, particularly benzene [8]. On this basis, acetone produced from IPA may be preferred in the pharmaceutical industry due to substantial restrictions on solvent use [9]. Furthermore, IPA dehydrogenation is considered a clean and sustainable energy source for producing hydrogen [10].

Oxidative dehydrogenation methods of isopropyl alcohol in the vapor phase are usually carried out with the help of catalysts, such as copper, silver, nickel, and platinum. This process occurs at high temperatures, thus requiring large amounts of energy [1]. The applicable reaction for dehydrogenation of isopropyl alcohol is as follows [11].

$$C_3H_8O_{(g)} \rightarrow C_3H_6O_{(g)} + H_{2(g)} \quad \Delta H^\circ_{298} = 55.02\ \frac{\text{kJ}}{\text{mol}} \qquad (1)$$

Thermodynamically, the rate of alcohol dehydrogenation reaction is strongly influenced by the presence of hydrogen. In this case, copper becomes the catalyst of first choice due to its high selectivity towards the alcohol dehydrogenation reaction. Therefore, catalysts containing large amounts of copper are indispensable to improve production efficiency [12]. However, the current dehydrogenation process must include energy efficiency, posing economic sustainability challenges. In addition, achieving high conversion rates in acetone production is still challenging in this industry, limiting overall production [13].

This study will explore the design of an acetone plant using simulation, focusing on enhancing the purity of the acetone product and increasing energy efficiency. The study results show that implementing sustainable design at every stage of the process can be a solution to overcome this challenge. Moreover, efforts to optimize energy efficiency in the industrial sector are essential, aligning with the industry's key objectives.

2. Materials and Methods

A model of the acetone production process from the dehydrogenation of isopropyl alcohol can be designed using Aspen HYSYS V12, and the corresponding process flow sheet is depicted in Figure 1. This simulation model serves to predict the process response of a plant through the application of mass and energy balances, phase considerations, and chemical equilibrium relationships. Aspen HYSYS offers an accurate and comprehensive thermodynamic foundation for physical calculations, real-time operating conditions, and rigorous equipment models to mimic actual plant processes. Simulation of process equipment using HYSYS includes a complete library of unit operation models, including distillation, reactors, heat transfer operations, rotating equipment, controllers, and logical operations, in both steady-state and dynamic environments to meet market demands [14]. he model from this simulation can improve process efficiency by reducing energy consumption and increasing the purity of acetone production to industry standards. The production process information for acetone is sourced from the literature [12]. Then, to fulfill the market demand, it is important to increase the yield and purity of acetone from the dehydrogenation of isopropyl alcohol through the best process design. The first stage, conceptual design, aims to determine the optimal process flow. Alternative designs are selected based on economic feasibility, environmental constraints, and utility efficiency, based on steps including flow charts, process calculations, equipment sizing, cost analysis, and calculating the energy requirements used [15].

Modification of the isopropyl alcohol (IPA) dehydrogenation process was carried out to increase acetone production yield while lowering energy requirements. In this modification, the pump was removed from the system, and a heat

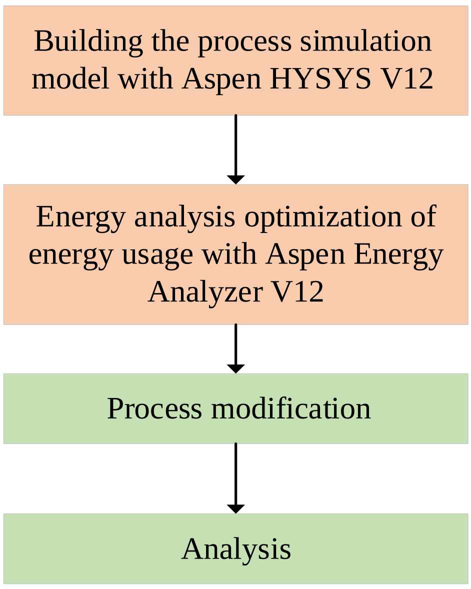


Figure 1. Process integration methodology chart.

exchanger was added to utilize the reactor output heat to increase the feed temperature. The operating temperature of the reactor was increased from 350 °C to 500 °C to improve reaction efficiency. In the reference process flow diagram (PFD), the system uses two coolers for cooling. However, in this modification, one of the coolers is replaced with a heat exchanger (HE) that utilizes the separator output temperature to cool the feed coming from the compressor. This change aims to maximize acetone production while reducing energy consumption in the system.

A conceptual process simulation model was developed specifically for the production of acetone via dehydrogenation of isopropyl alcohol. Furthermore, the Aspen Energy Analyzer V12 tool was used to analyze the energy consumption throughout the plant process. Aspen HYSYS was applied to optimize energy efficiency and heat transfer and conversion studies on acetone production. Detailed simulations included measurement operations that represented the real-time concept of the plant's industrial processes.

3. Result and Discussion

3.1 Process Description and Simulation

The concepts described in the literature form the basis for acetone production with isopropyl alcohol (IPA) dehydrogenation [12]. Figure 2 shows an industrial-scale isopropyl alcohol dehydrogenation plant designed to produce Acetone as the main product. The simulation model of this process was designed using Microsoft Visio. The reactor used is a Gibs reactor operating at 350 ℃ with a pressure of 1 bar. The NRTL thermodynamic model was selected to account for the various phases that may occur in this process.

The feed, which is isopropyl alcohol, is mixed with the recycle stream from the rest of the previous process. This stage aims to ensure homogeneity of the mixture before further processing. The mixture is then pumped to increase its pressure and heated to a high temperature in preparation for entering the reactor [16].

In the reaction stage, IPA is d dehydrogenated in a reactor under specific operating conditions: high temperature and controlled pressure. This endothermic reaction produces acetone as the main product and hydrogen as a by-product [17]. The reactor output product as a gas mixture is then cooled gradually to reduce its temperature to suit the following separation process. After cooling, the high-pressure gas separates hydrogen as a gas, while the liquid product containing acetone and residual IPA is sent for further purification.

The liquid product is then reheated before being fed into the distillation column. At the distillation stage, separation is carried out based on the components' boiling points [18]. Acetone, as the main product with a boiling point of 329.22 K at a pressure of 0.1 MPa, is separated from the remaining IPA, which has a boiling point of 355.5 K at a pressure of 0.1 MPa in the distillation column [19]. The top product of the distillation column is pure acetone with high purity. In contrast, the remaining IPA, which still contains a small amount of acetone, is returned to the initial stage of the process for recycling.

This process was simulated using Aspen HYSYS 12 software to model the material and energy flows in the system, as shown in Figure 3.

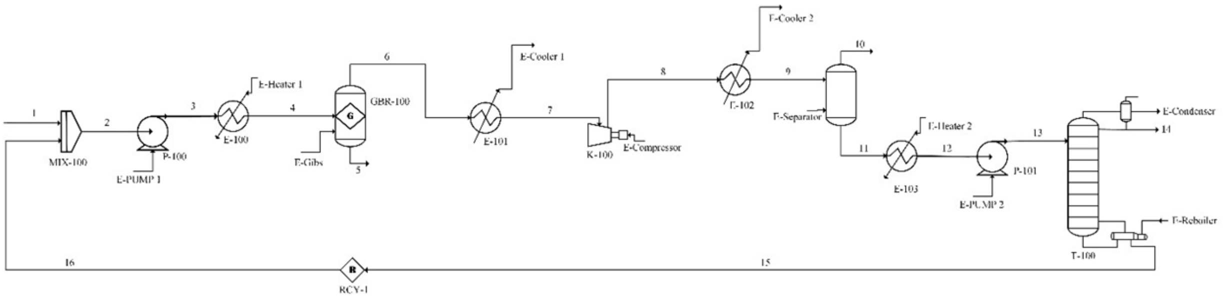


Figure 2. Basic process flow diagram for acetone production [12]

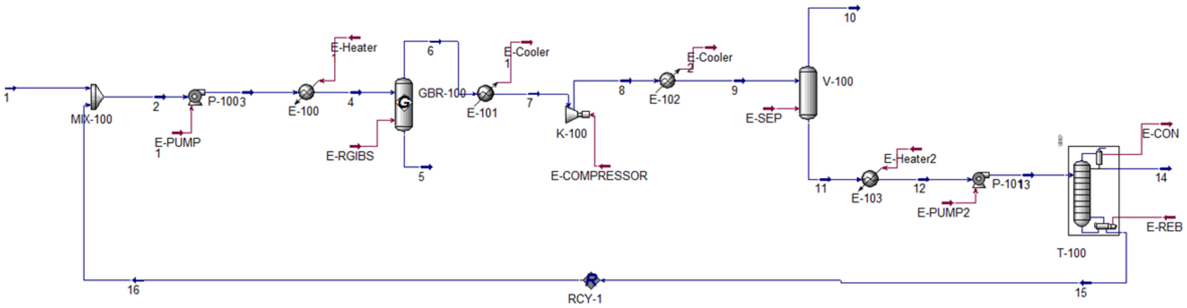


Figure 3. Aspen HYSYS simulation model for basic acetone production process

The NRTL equation was chosen because it can calculate multiple phases. At the initial stage, the raw material mixture is fed into the mixer unit (MIX-100) and flowed to the pump (P-100) to increase its pressure to 2 bar. Next, the flow is heated in the first heater (E-100) to raise its temperature to 350 °C before entering the gibs reactor (GBR-100). The dehydrogenation reaction occurs at 350 °C and 1 bar pressure in the reactor. This reactor produces a gas mixture of acetone, hydrogen, and residual isopropanol (IPA). The gas mixture then undergoes a two-stage cooling process.

The gas mixture is cooled in the first stage using a cooler (E-101). Next, the gas is compressed using a compressor (K-100) to increase its pressure to 12 bar. This compression process causes the gas temperature to increase to 196 °C. Therefore, the gas is cooled again using a cooler (E-102) until it reaches a temperature of 5 °C. After cooling, the gas mixture is separated in the separator (V-100). The separation results show that hydrogen is a product in the gas phase, while acetone and the rest of the IPA are in the liquid phase.

The liquid product from the separator is then heated in the second heater (E-103). After heating, the second pump (P-101) increases the liquid product pressure. The liquid then flows to the distillation column (T-100) for separation at a temperature of 154.6 °C and a pressure of 9.5 bar.

The upper distillation product, pure acetone, is shown in stream 14, with an acetone composition of 3078.2160 kg/h. The remaining IPA, along with a small amount of acetone, is returned to the mixing unit (MIX-100) as a recycle stream. The simulation results are shown in Table 1.

3.2 Thermodynamics and Operating Conditions Consideration

From a thermodynamic point of view, based on the enthalpy value of the formation reaction, it is endothermic and irreversible. Table 2 shows the values of ($\Delta H°_f$) and ($\Delta G°_f$) of each component at 298 K [20].

Reaction:

$$C_3H_8O_{(g)} \rightarrow C_3H_6O_{(g)}+H_{2(g)}$$

$$\Delta H_{r°} = \Delta H_{f°produk} - \Delta H_{f°reaktan}$$

$$\Delta H_{r°} = (\Delta H_f° \ C_3H_6O + \Delta H_f° \ H_2)$$

$$- (\Delta H_f° \ C_3H_8O)$$

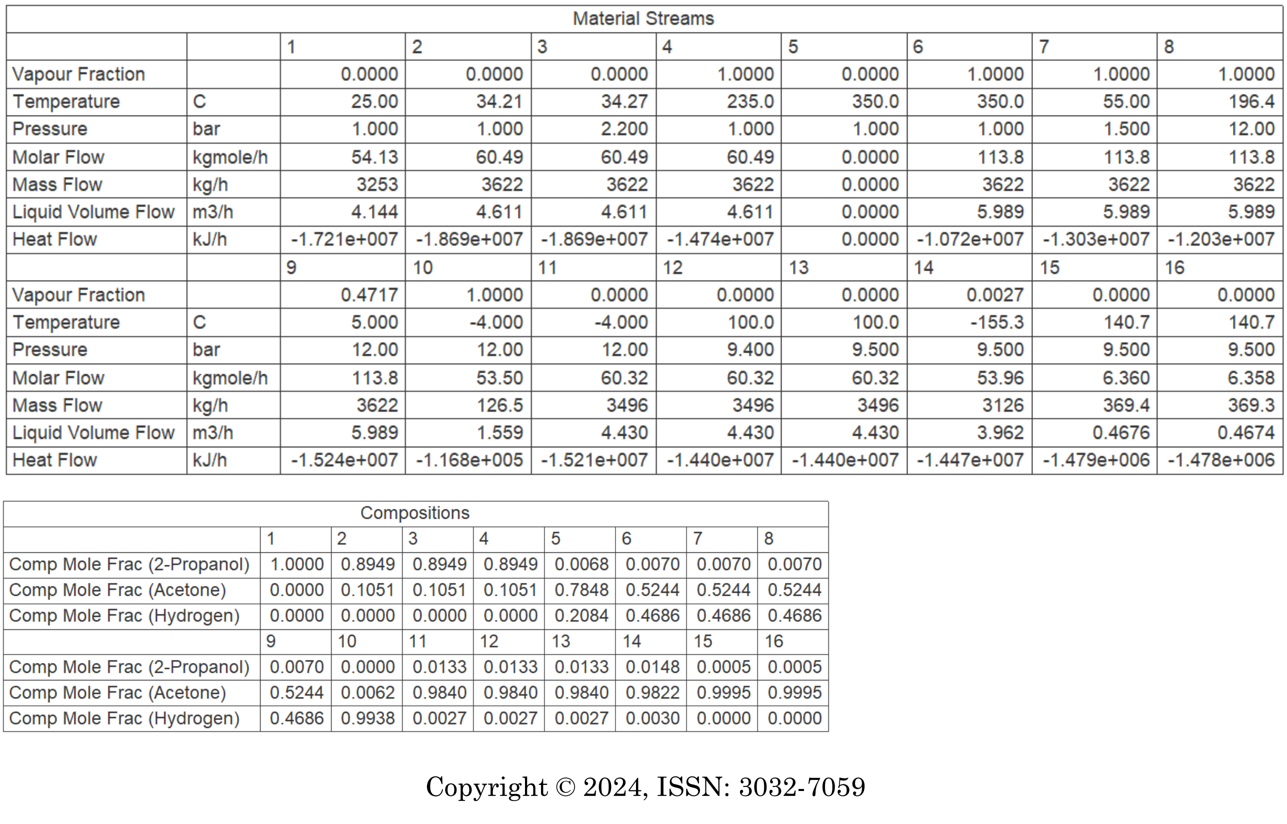
$$\Delta H_{r°} = (-217.57 + 0) - (-271.59)$$

$$\Delta H_{r°} = 55.02 \frac{kJ}{mol} = 55020 \frac{J}{mol}$$

Table 2. Gibs value ($\Delta G_f°$) and standard enthalpy ($\Delta H_f°$)

Component	(ΔHf°) (kJ/mol)	(ΔGf°) (kJ/mol)
C_3H_8O	-272.59	-173.59
C_3H_6O	-217.57	-153.05
H_2	-	-

Table 1. Mass and energy balances of the basic process for acetone production



Material Streams									
		1	2	3	4	5	6	7	8
Vapour Fraction		0.0000	0.0000	0.0000	1.0000	0.0000	1.0000	1.0000	1.0000
Temperature	C	25.00	34.21	34.27	235.0	350.0	350.0	55.00	196.4
Pressure	bar	1.000	1.000	2.200	1.000	1.000	1.000	1.500	12.00
Molar Flow	kgmole/h	54.13	60.49	60.49	60.49	0.0000	113.8	113.8	113.8
Mass Flow	kg/h	3253	3622	3622	3622	0.0000	3622	3622	3622
Liquid Volume Flow	m3/h	4.144	4.611	4.611	4.611	0.0000	5.989	5.989	5.989
Heat Flow	kJ/h	-1.721e+007	-1.869e+007	-1.869e+007	-1.474e+007	0.0000	-1.072e+007	-1.303e+007	-1.203e+007
		9	10	11	12	13	14	15	16
Vapour Fraction		0.4717	1.0000	0.0000	0.0000	0.0000	0.0027	0.0000	0.0000
Temperature	C	5.000	-4.000	-4.000	100.0	100.0	-155.3	140.7	140.7
Pressure	bar	12.00	12.00	12.00	9.400	9.500	9.500	9.500	9.500
Molar Flow	kgmole/h	113.8	53.50	60.32	60.32	60.32	53.96	6.360	6.358
Mass Flow	kg/h	3622	126.5	3496	3496	3496	3126	369.4	369.3
Liquid Volume Flow	m3/h	5.989	1.559	4.430	4.430	4.430	3.962	0.4676	0.4674
Heat Flow	kJ/h	-1.524e+007	-1.168e+005	-1.521e+007	-1.440e+007	-1.440e+007	-1.447e+007	-1.479e+006	-1.478e+006

Compositions								
	1	2	3	4	5	6	7	8
Comp Mole Frac (2-Propanol)	1.0000	0.8949	0.8949	0.8949	0.0068	0.0070	0.0070	0.0070
Comp Mole Frac (Acetone)	0.0000	0.1051	0.1051	0.1051	0.7848	0.5244	0.5244	0.5244
Comp Mole Frac (Hydrogen)	0.0000	0.0000	0.0000	0.0000	0.2084	0.4686	0.4686	0.4686
	9	10	11	12	13	14	15	16
Comp Mole Frac (2-Propanol)	0.0070	0.0000	0.0133	0.0133	0.0133	0.0148	0.0005	0.0005
Comp Mole Frac (Acetone)	0.5244	0.0062	0.9840	0.9840	0.9840	0.9822	0.9995	0.9995
Comp Mole Frac (Hydrogen)	0.4686	0.9938	0.0027	0.0027	0.0027	0.0030	0.0000	0.0000

The reaction that occurs is endothermic because the enthalpy value of the reaction is positive, so the reaction captures heat.

$$\Delta G_{298\text{K}} = \Delta G_{\text{f}^\circ\text{produk}} - \Delta G_{\text{f}^\circ\text{reaktan}}$$
$$\Delta G_{298\text{K}} = \left(\Delta G_{\text{f}^\circ C_3H_6O} + \Delta G_{\text{f}^\circ H_2}\right) - \left(\Delta G_{\text{f}^\circ C_3H_8O}\right)\Delta G_{298\text{K}}$$
$$= (-153.05 + 0) - (-173.59)$$
$$\Delta G_{298\text{K}} = 20.54\,\frac{\text{kJ}}{\text{mol}} = 20540\,\frac{\text{J}}{\text{mol}}$$

Based on the Van't Hoff equation [21]:

$$\ln K \;=\; \frac{-\Delta G_{298\text{k}}}{\text{R}T_{298}}$$
$$\ln K \;=\; \frac{-20.540\,\frac{\text{J}}{\text{mol}}}{8.314\,\frac{\text{J}}{\text{mol.K}} \times 298\text{K}}$$
$$K_{298\text{k}} = 2.51 \times 10^{-3}$$

To determine the value of K at an operating temperature of 500 °C (773 K) can be done in the following way:

$$\ln\left(\frac{K_{773\text{K}}}{K_{298\text{K}}}\right) = \frac{-\Delta H_{\text{r}^\circ}}{\text{R}}\left(\frac{1}{T_{773}} - \frac{1}{T_{298}}\right)$$
$$K_{773\text{K}} \;=\; 2.1181631 \times 10^{3}$$

The value of the reaction equilibrium constant at 500 °C (773 K) is less than one, so the reaction is irreversible.

3.3 Increased Product Purity by Process Modification

In general, acetone production through this process can still improve efficiency and purity. Thermal energy integration is an important aspect of maximizing heat recovery and optimizing utility design in the system to achieve better energy efficiency. This study was conducted using Aspen Energy Analyzer, where the required data, including the hot and cold streams of the entire process, were obtained through Aspen HYSYS. Process modifications were made to develop a more efficient acetone production process design that produces high purity, as shown in Figures 4 and 5.

The design modification of the acetone process involves the same initial steps as the basic process system. The differences and innovations

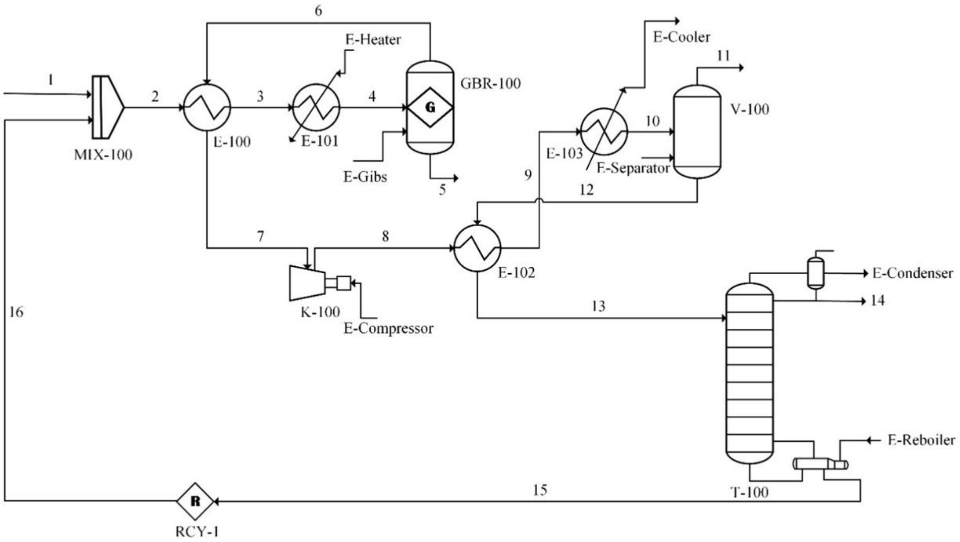


Figure 4. Modified process flow diagram for acetone production

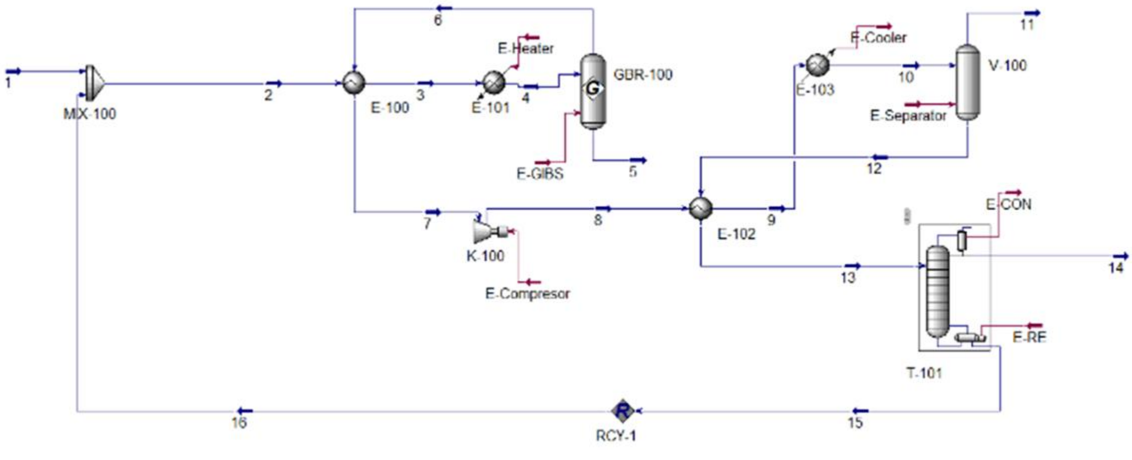


Figure 5. Aspen HYSYS simulation model for modified acetone production process

in this process are found in the reactor operating conditions, heating, and cooling. In the reactor operating conditions, the reactor temperature in GBR-100 was increased from the previous reactor temperature to 500 °C. This aims to increase the conversion from reactants to products [22]. As for heating and cooling, a heat exchanger uses counterflow to increase energy efficiency in the process system because it can minimize external energy requirements compared to heaters and coolers that require additional energy supply [23]. The final product of this process is represented in flow 14, with an acetone mass of 3117.9298 kg/h. The simulation results are shown in Table 3.

This process design modification integrates the concept of higher product purity compared with the previous acetone process design. In addition, the acetone product's mass is higher than that of the basic process system. The next chapter will discuss further comparison of the process design in terms of energy and purity.

3.4 Product Purity Analysis

The quality of the acetone product serves as an indicator for both the plant and the overall quality of the product produced. A higher level of purity in the product indicates superior quality, both for the product itself and the factory [24]. To determine the percentage of purity in the two simulation processes, the calculation is carried out using the Equation below [25]:

$$\%\text{Purity} = \frac{\text{mass of acetone product}}{\text{total product mass}} \times 100\% \quad (2)$$

The mass of acetone and the mass of the total product were obtained from Aspen HYSYS simulation data. Table 4 interprets the data for the total product mass in the basic process design. Using the data in Table 4, the calculation of acetone purity in the basic process system according to Equation (2) is as follows:

%Purity of basic process =

$$= \frac{3078.2160\ (\frac{\text{kg}}{\text{h}})}{3126.4145\ (\frac{\text{kg}}{\text{h}})} \text{x}100\%$$

$$= 98.46\%$$

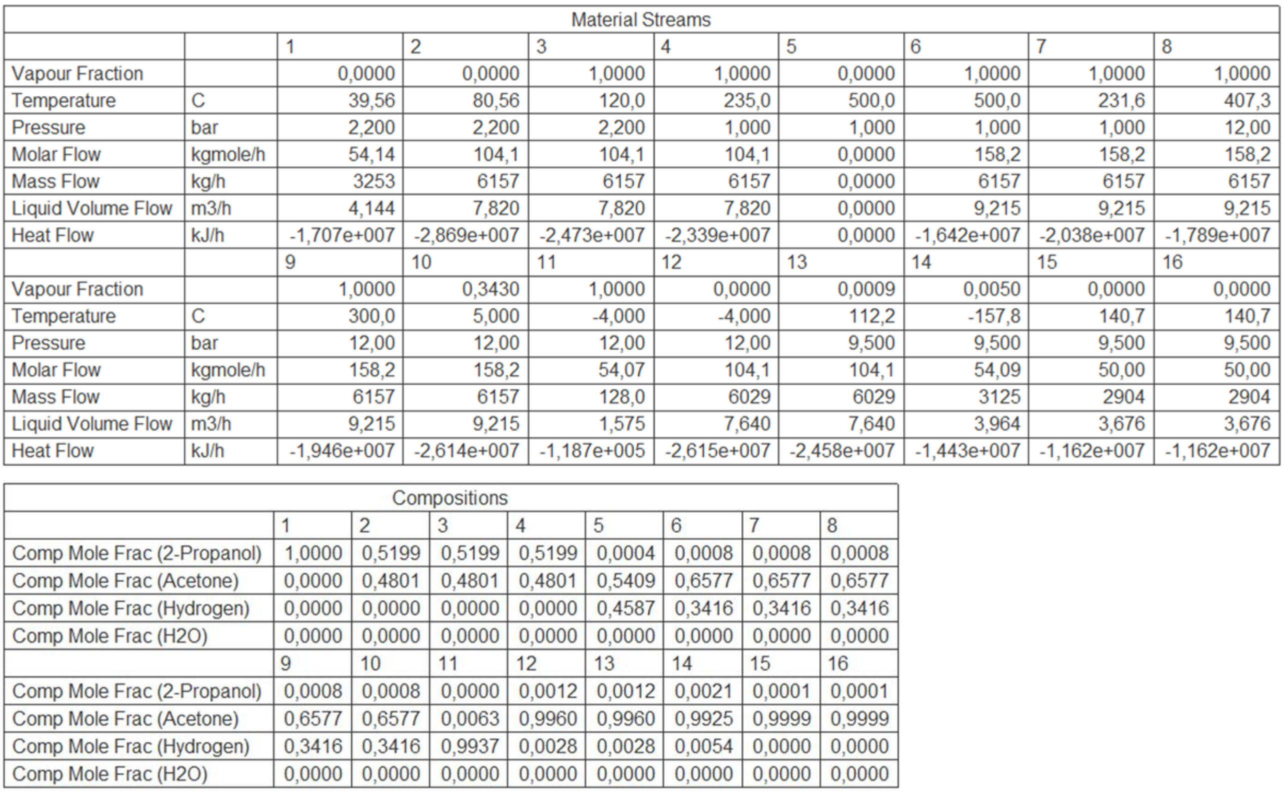
Based on these calculations, acetone produced using the basic process system has a purity of 98.46%. The purity of methyl chloride in the modified process was also calculated using the same method to compare with the modified process. Table 5 shows the mass of methyl chloride product obtained from the modified process.

%Purity of modified process =

$$= \frac{3117.9298\ (\frac{\text{kg}}{\text{h}})}{3125.3301(\frac{\text{kg}}{\text{h}})} \text{x}100\%$$

$$= 99.76\%$$

Table 3. Mass and energy balances of the modified acetone production process



Material Streams

		1	2	3	4	5	6	7	8
Vapour Fraction		0,0000	0,0000	1,0000	1,0000	0,0000	1,0000	1,0000	1,0000
Temperature	C	39,56	80,56	120,0	235,0	500,0	500,0	231,6	407,3
Pressure	bar	2,200	2,200	2,200	1,000	1,000	1,000	1,000	12,00
Molar Flow	kgmole/h	54,14	104,1	104,1	104,1	0,0000	158,2	158,2	158,2
Mass Flow	kg/h	3253	6157	6157	6157	0,0000	6157	6157	6157
Liquid Volume Flow	m3/h	4,144	7,820	7,820	7,820	0,0000	9,215	9,215	9,215
Heat Flow	kJ/h	-1,707e+007	-2,869e+007	-2,473e+007	-2,339e+007	0,0000	-1,642e+007	-2,038e+007	-1,789e+007
		9	10	11	12	13	14	15	16
Vapour Fraction		1,0000	0,3430	1,0000	0,0000	0,0009	0,0050	0,0000	0,0000
Temperature	C	300,0	5,000	-4,000	-4,000	112,2	-157,8	140,7	140,7
Pressure	bar	12,00	12,00	12,00	12,00	9,500	9,500	9,500	9,500
Molar Flow	kgmole/h	158,2	158,2	54,07	104,1	104,1	54,09	50,00	50,00
Mass Flow	kg/h	6157	6157	128,0	6029	6029	3125	2904	2904
Liquid Volume Flow	m3/h	9,215	9,215	1,575	7,640	7,640	3,964	3,676	3,676
Heat Flow	kJ/h	-1,946e+007	-2,614e+007	-1,187e+005	-2,615e+007	-2,458e+007	-1,443e+007	-1,162e+007	-1,162e+007

Compositions

	1	2	3	4	5	6	7	8
Comp Mole Frac (2-Propanol)	1,0000	0,5199	0,5199	0,5199	0,0004	0,0008	0,0008	0,0008
Comp Mole Frac (Acetone)	0,0000	0,4801	0,4801	0,4801	0,5409	0,6577	0,6577	0,6577
Comp Mole Frac (Hydrogen)	0,0000	0,0000	0,0000	0,0000	0,4587	0,3416	0,3416	0,3416
Comp Mole Frac (H2O)	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000
	9	10	11	12	13	14	15	16
Comp Mole Frac (2-Propanol)	0,0008	0,0008	0,0000	0,0012	0,0012	0,0021	0,0001	0,0001
Comp Mole Frac (Acetone)	0,6577	0,6577	0,0063	0,9960	0,9960	0,9925	0,9999	0,9999
Comp Mole Frac (Hydrogen)	0,3416	0,3416	0,9937	0,0028	0,0028	0,0054	0,0000	0,0000
Comp Mole Frac (H2O)	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000	0,0000

Based on the purity data between the basic acetone production process system and the modified acetone production process (Table 6), it can be compared that acetone with the modified process has a higher purity of 99.76%, with a difference of 1.3% between the two processes.

3.5 Analysis of Energy Used in Utilities

Using the Aspen Energy Analyzer simulation, energy demand data was obtained for the basic acetone production process system and the modified acetone production process. Furthermore, a comparison of the energy requirements for each process is shown in Figure 6 and Figure 7.

Data analysis from Figure 6 and Figure 7 shows that the energy requirements for the basic process system are higher than those for the modified process. This can be seen from the more excellent value of energy requirements in the basic process system compared to the modified process. Regarding energy, the modified process system is much more efficient, with energy savings of 40.89%, compared to the basic process system, which had 32.96%. In addition, the modified process reduced carbon emissions by 40.88%, better than the basic process, which had 32.96%. Thus, the modified process can be considered more environmentally friendly than the basic process system.

4. Conclusion

The modification of the isopropyl alcohol (IPA) dehydrogenation process successfully increased the purity of acetone from 98.46% in the original process to 99.76% in the modified version. Additionally, energy consumption in the modified process decreased by 40.89%, and there was a significant reduction in carbon emissions by 40.88% compared to the baseline process, where both energy consumption and carbon emissions were at 32.96%. These results indicate that the modified process is not only more efficient but also more environmentally friendly than the initial setup. However, the economic evaluation of this modification has not been addressed in this study. Future research should assess the financial feasibility of this modification using tools such as the Aspen Process Economic Analyzer (APEA) to gain deeper insights into the industrial scalability and application of this improved process.

Table 4. Composition of basic process system product

Composition	Mass flow (kg/h)
Isopropanol alcohol	47.8670
Aceton	3078.2160
Hydrogen	0.3315
Total product	3126.4145

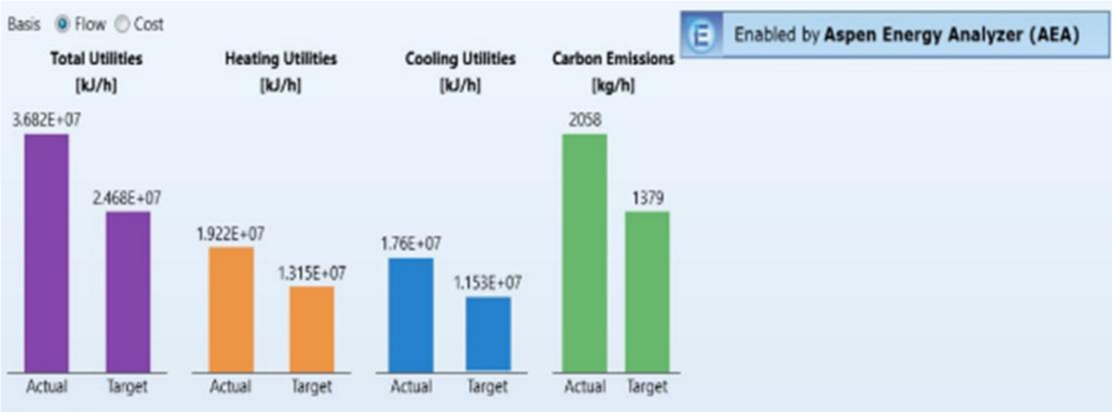


Figure 6. Energy requirements in the acetone basic process system

Table 5. Composition of modification process system product

Composition	Mass flow (kg/hour)
Isopropanol alcohol	6.8106
Aceton	3117.9298
Hydrogen	0.5897
Total product	3125.3301

Table 6. Comparison of acetone purity between basic and modified process flow diagrams

Purity of methyl chloride base process system production (%)	Purity of methyl chloride production with modification process (%)
98.46	99.76
Residual	1.3

Credit Author Statement

Author Contributions: A. K. Cahyaningtyas: Resources, Writing - Original Draft, Writing - Review and Editing, Visualization, Supervision; J. Zakariya: Conceptualization, Methodology, Formal Analysis, Data Curation, Writing - Original Draft, Writing - Review, Visualization, Software, Project Administration; M. A. Fahrozi: Conceptualization, Methodology, Validation, Writing - Original Draft, Writing – Review, Formal Analysis, Supervision; M. S. Hazim: Conceptualization, Methodology, Investigation, Resources, Writing - Original Draft; Y. K. Ariqah: Methodology, Validation, Resoruces, Writing - Original Draft, Writing – Review, Visualization, Supervision. All authors have read and agreed to the published version of the manuscript.

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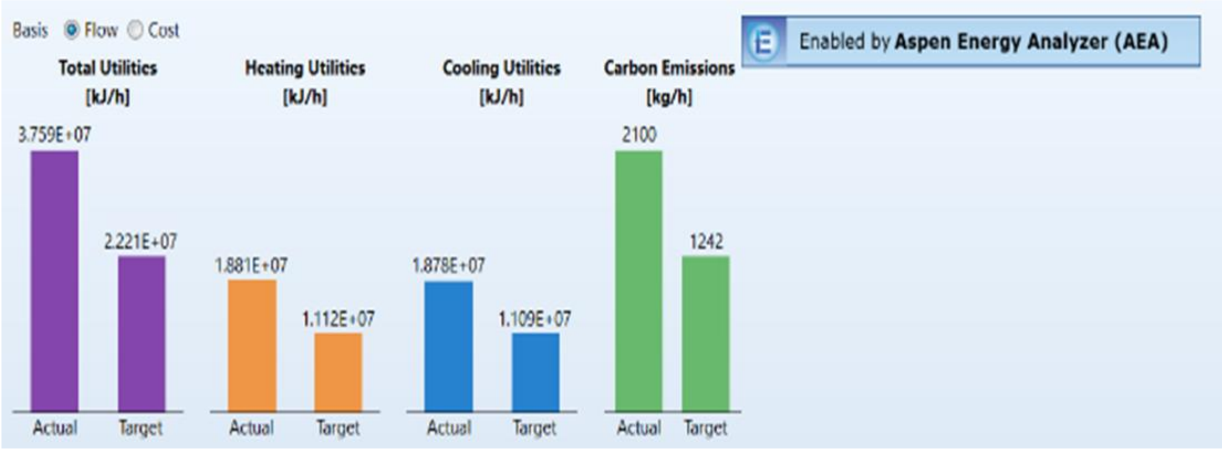

Figure 7. Energy requirement in the modified acetone process

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