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Research Article

Optimizing The Net Energy of Acetone Production using The Isopropyl Alcohol Dehydrogenation Process

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Abstract

In order to reduce the dependence on fossil fuels, acetone has emerged as an important platform chemical for various industrial applications. Acetone can be efficiently produced through the dehydrogenation of isopropanol, using metal-based catalysts with high activity and selectivity. The technology for this acetone production was simulated using Aspen HYSYS software, with operating parameters based on the reaction dynamics model for isopropanol dehydrogenation. This study evaluated the modification of the dehydrogenation process to improve energy efficiency by optimizing the heat transfer unit. The product heat leaving the reactor will be cooled in a heat exchanger and the heat is used to increase the heat from the mixer output, this is designed to utilize the process output energy, thus utilizing the heat exchanger as a cooler for the reactor output, thereby reducing additional energy consumption and improving the overall process sustainability. The modification includes increasing the acetone production yield and energy efficiency in the heat transfer unit to reduce energy consumption from 10.9296 MMBtu/h to 7.7431 MMBtu/h by utilizing the heat exchanger as a cooler for the reactor output back and at the same time a heater for the mixer output as a process optimization.

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Keywords: Acetone; Isopropanol; Simulation; Aspen HYSYS; Net energy

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1. Introduction

Acetone is a by product generated through the cumene process for phenol production. The increasing demand for phenol, driven by its use in phenolic resins and polycarbonates, has resulted in an excess of acetone, with a global surplus estimated at 1.7 million tons. To enhance the economic viability of the process, upgrading acetone into more valuable products is essential. Catalytic hydrogenation of acetone, conducted in both vapor and liquid phases, has long been studied for the production of isopropyl alcohol (IPA). IPA serves as a versatile solvent and a key chemical intermediate across industries, including paints, inks, electronics, food, and pharmaceuticals. Additionally, it is used to produce chemical derivatives like isopropyl ethers, esters, and amines. Furthermore, IPA can be utilized in the production of cumene through benzene alkylation, reducing the reliance on petroleum-derived propylene for phenol manufacturing [1].

Acetone consists of a ketone functional group and two identical alkyl groups, namely methyl groups on both sides of the ketone functional group, giving it the chemical formula CH_3COCH_3

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and a molecular weight of 58.08 g/mol. Acetone, also known as propanone, dimethyl ketone, or 2-propanone, is an organic compound composed of three carbon atoms and is the simplest, most basic, and earliest discovered compound in the ketone group [2].

Acetone was first identified by chemists in the late medieval period through the dry distillation of acetate salts such as lead acetate. French chemist Jean Baptiste André Dumas and German chemist Justus Freiherr von Liebig successfully determined the experimental chemical formula for this compound in 1832. Acetone is an important industrial solvent and is often considered the solvent of choice for laboratory cleaning. In large quantities, acetone is used across various industries, including dye, plastic, fiber, and pharmaceutical industries. It is also used as a solvent in certain cleaning agents and other chemical products [2].

Acetone can be produced through several methods, including the cumene hydroperoxide process, isopropanol dehydrogenation, and isopropanol oxidation. One of the most important methods is the isopropyl alcohol (isopropanol) dehydrogenation process, which involves catalytic dehydrogenation in an endothermic reaction as follows:

$$CH_3CHOHCH_3 \longrightarrow CH_3COCH_3 + H_2 \qquad (1)$$
$$\Delta H^o_{f298k} = 104900 \text{ J/mol}$$

In this process, isopropyl alcohol is vaporized using a vaporizer, heated in a heat exchanger with steam, and then fed into the reactor. This method is chosen for several reasons, including the absence of a need for an oxygen separation unit from air before being fed into the reactor, higher conversion rates resulting in greater acetone yields, and a lower likelihood of corrosion [3].

Acetone, being the simplest ketone compound, has numerous applications in various industrial fields. The demand for acetone in Indonesia continues to rise over time. However, to date, only a few factories in Indonesia produce acetone. Most acetone in the country is still imported from other countries, such as the United States, the Netherlands, China, South Korea, Japan, Malaysia, and Singapore.

Many modification have been made in simulation process for isopropyl alcohol dehydrogenation process, reactor model, and reaction operational condition in order to increase the acetone production has already been performed. As an improvement on existing methods, the design and simulation will be carried out numerically using Aspen HYSYS software. In this study, the technological process for the isopropyl alcohol dehydrogenation process is simulated in Aspen HYSYS based on the combined operating parameters of the reaction dynamic.

2. Methods

2.1 Process Simulators used for Evaluation

The process simulators we used for our process is Aspen HYSYS. Aspen HYSYS is very packages capable of solving complex tasks related to process engineering and give chemical engineers the opportunity to make fast and complex calculations [4]. Methods for producing acetone with isopropyl dehydrogenation, and using the Aspen HYSYS simulator tool.

The Aspen HYSYS is a process simulation environment designed to serve many processing industries. When it comes to the oil and gas and refining sectors for precise computation of physical characteristics, transport parameters, and phase behaviour [5]. It's an interactive, open and extensible program. Aspen HYSYS also has many add-on option to extend it's capability into specific industries. Rigorous steady state and dynamic models for plant design can be created from this program. Also, monitoring, troubleshooting, & operational improvement can be performed with this process simulator. Through it's completely interactive interface, process variable and unit operation topology can be easily manipulated [6]. Aspen HYSYS offers a comprehensive thermodynamics foundation for accurate calculation of physical properties, transport properties, and phase behaviour for the oil & gas and refining industries. Comprehensive library unit operation models is available including distillation, reactors, heat transfer operation, rotating equipment's, controllers and logical operations in both the steady state and dynamic environments [7].

2.2 Basic Process Flow Diagram from Literature

Figure 1 shows process flow diagram of acetone production plant. Isopropanol (IPA) stored in tank (Tank-01) at 30 ^oC and atmospheric pressure condition. In raw material preparation unit, isopropanol pressure is adjusted to 2 atm and vaporized [8]. Vaporizer product is then separated using flash drum, the top product in the form of vapor is then heated to a temperature of 101-350 ^oC, meanwhile the bottom product is recycled to be mixed again with fresh isopropanol feed [3]. The Acetone synthesis process is carried out in a multitube fixed bed reactor [9] The plug flow reactor operates at 350 °C with Dowtherm A as the heating medium and ZnO as the catalyst. Isopropanol is flowed through the reactor tube which acts as a plug flow and contains a ZnO catalyst, allowing the decomposition of isopropanol into acetone and H_2. This reaction

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achieves a conversion rate of 99.99%, with the reactor products consisting of acetone, H_2, air, and isopropanol in the vapor phase[10].

The reactor product stream in then cooled to 170 °C and condensed at temperature 30 °C to form vapor-liquid mixture. This mixture is then separated using separator (SP-02), the top product of SP-02 is directed to absorber (AB-01), while residual propanol and acetone are absorbed using water as solvent [11]. The bottom product of SP-02 is directed to mixing mount (MP-02.) The top result of AB-01 is hydrogen gas and a little acetone. The bottom result is acetone, water, and isopropanol which are then mixed with the bottom result of SP-02 in MP-02. The mixture is separated using a distillation column (MD-01). The MD-01 feed is first heated to 64 °C in HE-02. The top result of MD-01 is desired as a product in the form of acetone with a purity of 90% by mass. Then cooled with C-03 to a temperature of 30 °C and flowed to T-02. The bottom result of MD-01 is water, isopropanol, and acetone which are separated from MD-02 [12]. The top product of MD-02, a mixture of isopropanol, water, and trace amounts of acetone, is recycled back to MP-01. Meanwhile, the bottom product of MD-02 is sent to the Waste Treatment Unit [3].

2.3 Strategy Modification Heat Transfer Unit

Modifications are made by changing the cooler into a heat exchanger aimed to improve energy efficiency for producing acetone. Heat exchanger, has two functions of heating and cooling [13], can be used to reduce utility consumption in chemical processes which can lead to reduced utility costs and energy consumption [14]. In a utility, energy conservation can be achieved by efficient use of energy which is associated with decreased energy consumption and/or reduced consumption of conventional energy sources that affect production costs. Therefore, heat exchanger networks that often result in trade-off between equipment and operating cost may represent the best design for energy efficiency for producing acetone in chemical process plants [15].

The study by Saari e*t al*. [16], showed that the use of primary heat exchangers in reactors can optimize energy consumption by utilizing the reactor's heat output for heating, thereby reducing external energy requirements and carbon emissions. Meanwhile, Anxionnaz *et al*. [17], integrated the functions of heating, cooling, power production, and energy storage in one system, which was shown to significantly improve energy efficiency through the reuse of residual energy. Although technologies such as solar heating and air heat exchangers require higher initial installation costs compared to conventional heaters, the long-term benefits of significantly lower operating costs and significant energy savings make them an efficient and sustainable choice [18]. Heat exchangers not only reduce thermal stress on components but also extend the service life of the system, making them an energy-efficient solution in a variety of industrial applications [19]. With proper life-cycle cost analysis and environmental concerns, these technologies can reduce carbon impact while offering long-term cost efficiency, although challenges such as initial costs and installation complexity still need attention [20].

3. Results and Discussion

3.1 Basic Process Flow Diagram

Acetone plant is set at a production capacity of 8740 tons per year. Fluid packages of NRTL are applied to model the phase equilibrium of water and isopropanol system. Strong intermolecular force between isopropanol and water results in deviation from ideal behavior of phase equilibrium. NRTL is able to model the deviation

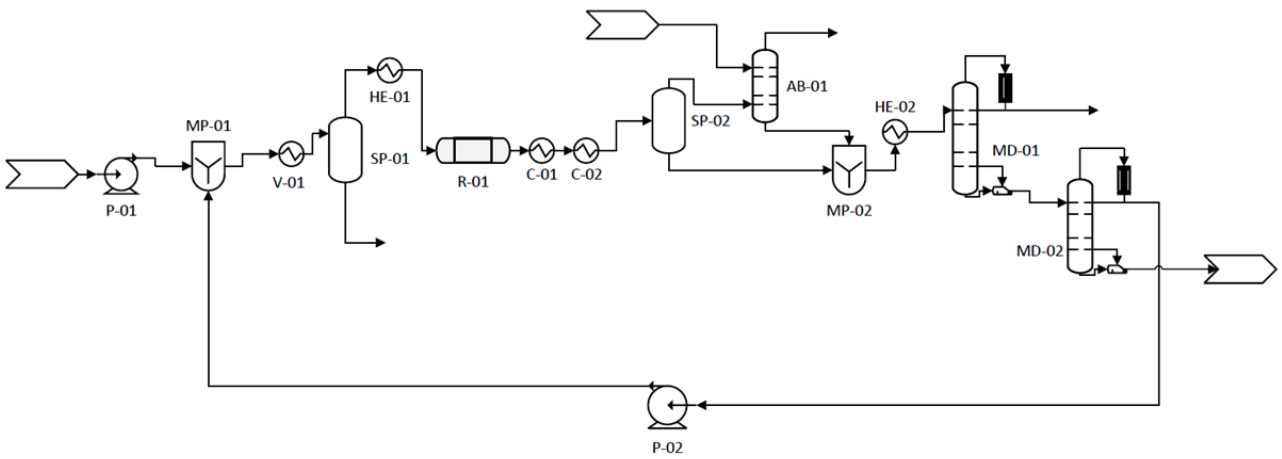

Figure 1. Process Flow Diagram (PFD) for the conversion of isopropyl alcohol to acetone

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by describing the interactions by random parameters [21].

Figure 2 shows process flow diagram of the basic/unmodified process of acetone production plant, while Figure 3 shows HYSYS simulation of the basic/unmodified process of acetone production plant. The dehydrogenation reaction of isopropanol is carried out in plug flow reactor at conditions 350 °C. Isopropanol (IPA) is introduced to the system at 30 °C , 1 atm, and 1312 kg/h with 70% purity (% wt). IPA stream pressure is then adjusted using pump (P-01) into 2 atm and then mixed by recycle stream from purification unit. The mixture is then vaporized using V-01 and separated using flash drum. Before entering the reactor, the mixture is heated into 350°C. The product of reactor is then cooled and condensed using cooler and condenser. This mixture is then separated using separator (SP-02), the top product of SP-02 is directed to absorber (AB-01), while residual propanol and acetone are absorbed using water as solvent The bottom product of SP-02 is directed to mixing mount (MP-02.). The top result of AB-01 is hydrogen gas and a little acetone.

The bottom result is acetone, water, and isopropanol which are then mixed with the bottom result of SP-02 in MP-02. The mixture is separated using a distillation column (MD-01). The MD-01 feed is first heated to 64 °C in HE-02. The top result of MD-01 is desired as a product in the form of acetone with a purity of 70% by mass. Then cooled with C-03 to a temperature of 30 °C and flowed to T-02. The bottom result of MD-01 is water, isopropanol, and acetone which are separated from MD-02. The top product of MD-02, a mixture of isopropanol, water, and trace amounts of acetone, is recycled back to MP-01. Meanwhile, the bottom product of MD-02 is sent to the Waste Treatment Unit.

3.2 Thermodynamics Consideration and Operating Conditions Consideration

Figure 4 shows process flow diagram of the modified process of acetone production plant, while Figure 5 presents Aspen HYSYS simulation of the modified process. According to Luyben, the manufacture of acetone from isopropanol through the dehydrogenation process is an endothermic reaction that requires external heat to occur. This process involves a ZnO catalyst and occurs in the gas phase at a temperature of 350 °C and a pressure of 2.3 atm, resulting in an isopropanol conversion of up to 90%. In accordance with the equilibrium theory, endothermic reactions require high temperatures to achieve optimal

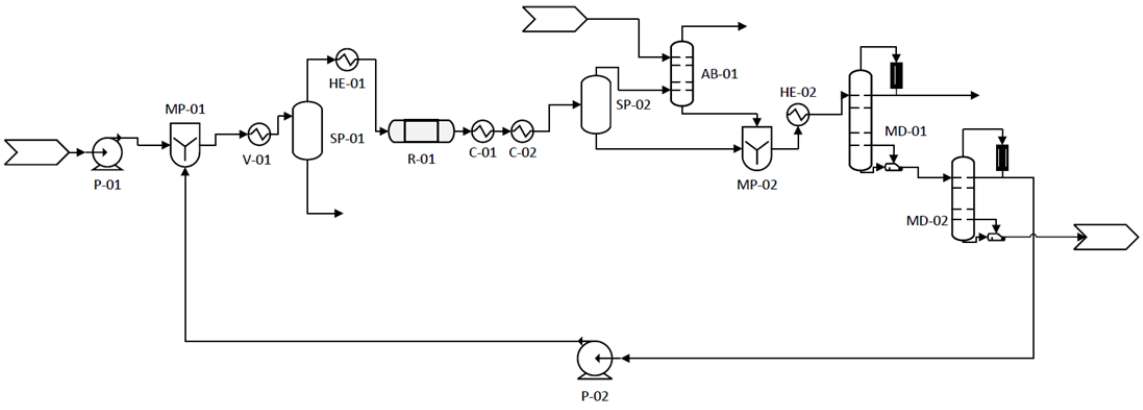

Figure 2. Process Flow Diagram (PFD) of basic process before process modifications

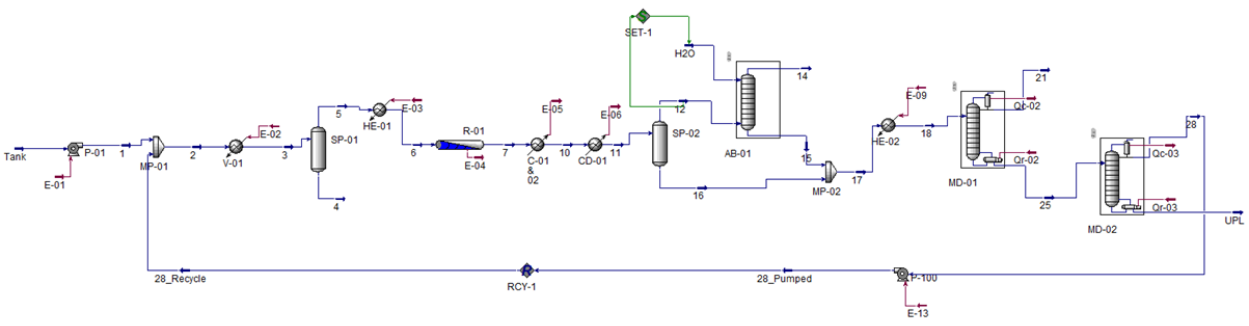

Figure 3. Aspen HYSYS simulation of basic process before modifications

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conversion, while decreasing the temperature will cause a decrease in conversion. Therefore, the reactor in this process is run isothermally with the help of a reactor heater in the form of steam to maintain a stable temperature and ensure that the reaction occurs efficiently. In addition, the nature of the endothermic reaction causes heat absorption during the reaction, so that temperature control is very important to maintain reaction equilibrium and conversion efficiency. A review of thermodynamics plays an important role in understanding the basic properties of the reaction, such as whether the reaction is endothermic or exothermic, as well as the direction of the equilibrium shift that determines whether the reaction is reversible or irreversible. Thermodynamic analysis also helps in determining the optimal operating conditions, such as temperature, pressure, and type of catalyst used, to maximize the energy efficiency and selectivity of acetone production. In addition, understanding the reaction enthalpy, Gibbs free energy change, and the influence of other thermodynamic factors is a crucial basis for designing an economical and sustainable system for industrial acetone production.

A thermodynamic review is used to determine the nature of the reaction, whether the reaction is exothermic or endothermic. In addition, the thermodynamic review is also used to determine the direction of the reaction shifting, whether the reaction is irreversible or reversible. Calculate the ΔH_{f298} value for the following isopropanol dehydrogenation reaction.

Heat of reaction ΔH^o_{f298k}

The data of 298 ΔH^o_{f298k} for each component in the isopropanol dehydrogenation is as follows :

$(CH_3)_2HOH \rightarrow (CH_3)_2CO + H_2$

$\Delta H^o_{f298k}(CH_3)_2HOH$ = -330.8 kJ/mol

$\Delta H^o_{f298K}\,(CH_3)_2CO$ = -4.2 kJ/mol
$\Delta H^o_{f298K}\,H_2$ = -221.7 kJ/mol
$\Delta H^o_{f298k} = \Delta H_{f\ product} - \Delta H_{f\ reactant}$
$\Delta H^o_{f298k} = (\Delta H_{f\ Aceton} + \Delta H_{f\ H_2}) - (\Delta H_{f\ isopropanol})$
= (-221.7 kJ/mol – 4.2 kJ/mol) – (-330.8 kJ/mol)
= 104900 J/mol

Based on the calculation, the ΔH value shows a positive value (+) so that the reaction is an endothermic reaction or a reaction that absorbs heat. If the operating temperature is higher, the conversion will be higher. Therefore, in order for the reaction to continue running according to operating conditions, heating is needed.

Gibbs Free Energy

The data of ΔG_{f298K} for each component in the isopropanol dehydrogenation process is as follows:
$\Delta G^o_{f298K}\,(CH_3)_2HOH$ = -185.2 kJ/mol
$\Delta G^o_{f298K}\,(CH_3)_2CO$ = 17.6 kJ/mol
$\Delta G^o_{f298K}\,H_2$ = -159.7 kJ/mol
$\Delta G^o_{f298} = \Delta G_{f,298K,\ product} - \Delta G_{f,298K,\ reactant}$
$= (\Delta G_{f\ Acetone} + \Delta G_{f\ H2}) - (\Delta G_{f\ isopropanol})$
= (-159.7 kj/mol +17.6 kJ/mol) – (-185.2 kJ/mol)
Therefore, ΔG^o_{f298K}= 43100 J/mol

From the Gibbs energy data, it can be seen that the value of ΔGf^o_{298K} is positive so that at an operating temperature of 298 K a catalyst is needed because the reaction is non-spontaneous. However, in this experiment, an operating temperature of 623 K or 350 ℃ will be used. In addition, to find out whether the reaction is reversible or irreversible, the following calculations are needed.

$$\ln K_{298} = \frac{-\Delta G^0}{RT} = \exp\left(\frac{-(43100)}{8{,}314\times298}\right)$$
$$K_{298} = 2.786 \times 10^{-8}$$

The K_{298} value obtained is 2.51×10^{-4}. However, because the operating temperature in this experiment is 350 ℃ or 623 K, it is necessary to calculate the K value at a temperature of 623 K which is explained as follows.

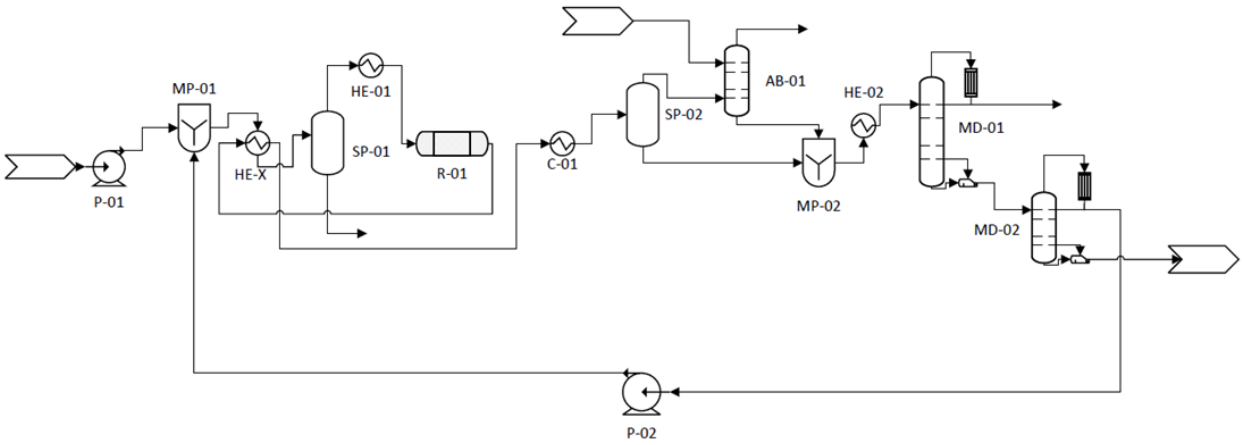

Figure 4. Process Flow Diagram (PFD) of modified process

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$\ln \frac{K_1}{K_{298}} = \frac{-\Delta H_{298}}{R}\left(\frac{1}{T} - \frac{1}{T_{298}}\right)$ $\ln \frac{K_1}{2.786\times10^{-8}} = \frac{-(104900\ \text{J/mol})}{8{,}314\ \text{J/mol.K}}\left(\frac{1}{623} - \frac{1}{298}\right)$

$K_1 = 108.2930$

To get the final K value, it is calculated in the following way.

$K = K_{298} \times K_1$

$K = 2.786 \times 10^{-8} \times 108.2930$

$K = 3.017 \times 10^{-6}$

The reaction equilibrium value at an operating temperature of 350 °C was obtained as 3.017×10^{-6} so that the reaction is an irreversible reaction.

3.3 Process Modification Impact

Heat recovery from the reactor product to heat and vaporize reactor feed results energy consumption reduction in the process. The replacement of vaporizer (V-01) and cooler (C-01 and C-02) reduces the heat duty required to vaporize and cool the stream in the process. The detailed result of process modification is shown in Table 1.

4. Conclusion

Simulation of a Acetone plant which is capable of producing Acetone (8740 ton/year) using the isopropyl alcohol dehydrogenation Process was done using Aspen HYSYS simulator. Fluid packages of NRTL are applied to model the phase equilibrium of water and isopropanol system. Energy consumption of simulation is reduced from 10.9296 MMBtu/h to 7.7431 MMBtu/h by utilizing the heat exchanger as a cooler for the reactor output back and at the same time a heater for the mixer output as a process optimization it was concluded that production of acetone from isopropyl alcohol dehydrogenation with lower net energy consumption is technically feasible. Further research into parameter changes and energy integration is necessary to optimize the process profitability.

CRediT Author Statement

Author contributions: A. N. Ihsan was responsible for conceptualization, methodology, visualization, writing, software development, review and editing, and validation. A. S. Wibawa contributed to conceptualization, investigation, visualization, project administration, writing, review and editing, as well as supervision. K. M. Ibrahim handled writing, review and editing, and also visualization. M. A. Kindi focused on investigation, methodology, software development, visualization, writing the original draft, and conducting reviews and edits. Finally, D. Ruliyono handled data curation, formal analysis, validation, and also overseeing supervision tasks. All authors have read and agreed to the published version of the manuscript.

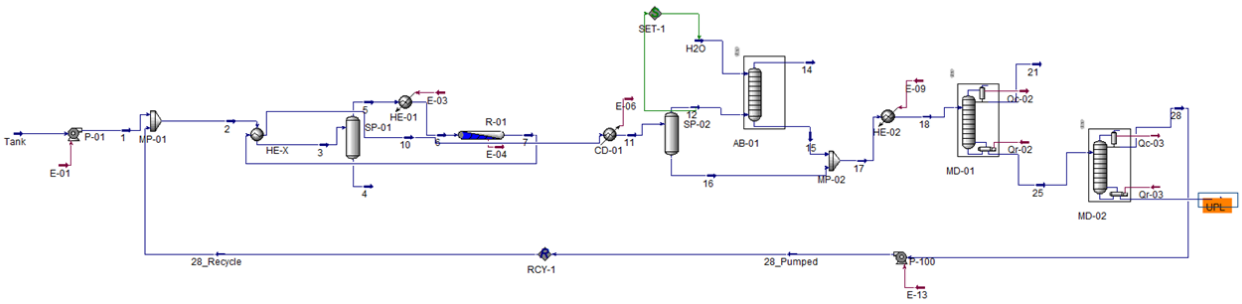

Figure 5. Aspen HYSYS simulation of the modified process

Table 1. Modification impact on overall duty required in acetone plant

Unit Operation	Unmodified	Modified
	MMBTU/h	
V-01	1.5773	
HE-01	0.9530	0.9569
C-01 & C-02	0.7382	
CD-01	1.3675	0.5271
HE-02	0.4575	0.5105
Reboiler Duty (MD-01)	1.6014	1.5386
Condenser Duty (MD-01)	2.2875	2.2772
Reboiler Duty (MD-02)	0.9733	0.9661
Condenser Duty (MD-02)	0.9738	0.9668
Total	10.9296	7.7431

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