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Research Article

Minimization of Energy Consumption Through Improving Purity of Hydrogen By-Product and Adding Heat Exchanger on Acetaldehyde Production Process

Abdurrahman Fawwaz*, Akbar Putra Ajie Nugraha, Muhammad Putra Al Rasyid, Refah Hakam Muhammad

Department of Chemical Engineering, Faculty of Engineering, Universitas Diponegoro, Semarang, Indonesia.

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Abstract

Improving energy efficiency in the acetaldehyde production process is one of the strategic steps to optimize operations and support the sustainability of the chemical industry. This study aims to analyze the impact of adding a heat exchanger and increasing the mass rate of the feed absorber (water) on energy efficiency and hydrogen purity, as a by-product. Simulations were conducted with thermodynamic modeling-based software to compare the unmodified process system with the modified system. The addition of a heat exchanger was designed to minimize heat energy loss in the system by recycling heat energy from the process stream. Meanwhile, increasing the mass rate of the feed absorber aims to increase the capacity of the water absorber in separating impurity compounds, thereby producing hydrogen with higher purity. Simulation results show that the system modified with the heat exchanger successfully reduces the total energy demand by 1,695,040.81 kJ/h. In addition, increasing the mass rate of the absorber feed significantly improves the hydrogen purity to reach a more optimal level for advanced applications. In conclusion, the combination of adding a heat exchanger and adjusting the mass rate of the feed absorber not only improves energy efficiency, but also provides added value in the form of hydrogen with higher purity. This study provides practical guidance for the development of a more efficient and environmentally friendly acetaldehyde production technology.

Keywords: Acetaldehyde; Energy Consumption; Purity Improvement; Hydrogen by Product; Energy Efficiency

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1. Introduction

Acetaldehyde (CH_3CHO) is a crucial petrochemical intermediate widely utilized in the synthesis of various chemicals, including acetic acid, pentaerythritol, acetic anhydride, and n-butanol. Under standard room conditions, acetaldehyde is characterized as a pungent and colorless liquid. The industrial production of acetaldehyde primarily involves three major processes: the oxidation of ethylene, hydration of acetylene, and dehydrogenation of ethanol. Among these methods, the dehydrogenation of ethanol stands out as a well-established and mature process that offers high selectivity for the main reaction while minimizing by-product formation [1].

The dehydrogenation of ethanol to produce acetaldehyde is particularly advantageous due to its operational simplicity and the moderate temperature and pressure conditions required. This process not only leads to a higher yield of acetaldehyde but also allows for easier purification though conventional unit operation, which are generally less complex and more cost-effective than those required for other production method. The aims of the process is to achieve a production target of 50.000 metric tons annually (MTA) with a purity level of at least 99.5 wt% The approximated flow rate of acetaldehyde product is

* Corresponding Author.
Email: abd.fawwazz18@gmail.com (A. Fawwaz)

6250 kg/h, assuming 8000 h of plant's annual operation. In addition, a by product of gaseous hydrogen with at least 95 wt% purity should be produced, while its production rate will be determined as part of the simulation exercise [2].

Energy optimization is critical in the production of acetaldehyde, particularly given the increasing global focus on sustainability and reducing carbon footprints in chemical manufacturing. Previous production often involve significant energy consumption due the high operational temperature and pressure. Therefore, enhancing energy efficiency not only reduces operational costs but also addresses environmental concerns associated with excessive energy use. Recent studies have highlighted innovative strategies such as integrating heat recovery system and optimizing reactor design to improve overall energy efficiency while maintaining high conversion rates [3]. In addition, the addition of heat exchangers plays a crucial role in optimizing the production process of acetaldehyde. Research has shown that the incorporation of heat exchangers can significantly enhance energy efficiency in acetaldehyde production while minimizing heat expenditure during production [4].

The novel contribution of this research lies in combining two approaches: first, the improvement of hydrogen purity through separation process optimization and second, the addition of heat exchangers to improve thermal efficiency in acetaldehyde production. In the oxidative process of ethanol dehydrogenation, we expect to achieve high selectivity towards acetaldehyde while reducing the required operating temperature. In addition, the use of a heat exchanger is expected to recover and utilize the energy wasted during the reaction, thus further reducing the overall energy consumption. Through this approach, it is expected that this research can make a significant contribution to the development of a more sustainable and energy-efficient acetaldehyde production process.

2. Methods

2.1 Property Package

Aspen HYSYS utilizes various thermodynamic equations, with the selection of suitable equations aimed at evaluating phase equilibrium and the enthalpy of mixed compounds. In this simulation of the dehydrogenation of ethanol process for acetaldehyde production, the NRTL [5] property package was employed.

2.2 Energy Optimization using Heat Exchanger

Heat transfer can be facilitated using heat exchangers, coolers, and heaters. Coolers and heaters function to absorb or supply energy to fluids by utilizing electricity or other energy sources [6]. In contrast, a heat exchanger transfers heat between two fluids without direct contact [7]. In the acetaldehyde production process, coolers and heaters are employed as heat transfer units. In the chemical industry, heat exchangers can reduce the amount of energy consumption by increasing or reducing fluid temperature using waste heat.

The dehydrogenation of ethanol process operates at high temperature [8]. So, before the ethanol feed enters the reactor, a heater must be added. To enhance energy efficiency in acetaldehyde production, a heat exchanger was selected. This heat exchanger makes use of the heat generated during the production process. This approach is feasible because the process involves both cooling and heating, allowing heat transfer between the two streams without requiring external energy input. The Specific Energy Consumption (SEC) [9] can be determined using the following equation:

$$SEC\left(\frac{kJ}{ton}\right) = \frac{Energy\ consumption \frac{kJ}{year}}{Production\ quantity \frac{ton}{year}} \quad (1)$$

2.3 Hydrogen Purity Improvement

Hydrogen is a by-product generated during the dehydrogenation of ethanol, a process that converts ethanol into acetaldehyde while releasing hydrogen as a reaction product. Initially, the produced hydrogen contains impurities as it is mixed with other gases, such as carbon dioxide and residual ethanol. To obtain pure hydrogen, purification steps are required, employing methods such as Pressure Swing Adsorption (PSA) [10], membrane separation [11], or chemical scrubbing [12]. The purified hydrogen holds significant potential for use as an environmentally friendly fuel or as a feedstock in various industrial applications, including ammonia synthesis [13] and catalytic hydrogenation [14].

The initial purity of hydrogen produced is often low due to the presence of impurities such as carbon dioxide, water vapor, or residual gases from the production process. To enhance the purity of the hydrogen, one effective approach is to adjust the mass flow rate of the absorbent used during the purification stage [15]. By optimizing the absorbent flow, the removal of impurities can be improved, allowing the hydrogen to reach a higher level of purity, which is essential for applications requiring clean and high-quality hydrogen.

3. Results and Discussion

3.1 Basic Process Flow Diagram of Acetaldehyde Production

Production Basic (unmodified) process flow diagram of acetaldehyde production is depicted in Figure 1, while Aspen HYSYS simulation of the basic process is depicted in Figure 2. Meanwhile, results of mass balance and energy balance (using Aspen HYSYS simulation) of the acetaldehyde production through the basic process of dehydrogenation of ethanol is presented in Table S1 (Supporting Information). The production of acetaldehyde begins with ethanol feedstock, which is pressurized using Pump 1 and preheated in Heater 1 before entering the reactor. The dehydrogenation of ethanol is carried out at temperatures around 300 °C to ensure sufficient activation energy for the reaction to proceed efficiently, as it is an endothermic process requiring heat input. At this temperature, the kinetic energy of ethanol molecules increases, promoting the breaking of C-H bonds and facilitating the formation of acetaldehyde and hydrogen [16]. Additionally, higher temperatures shift the equilibrium towards the products, as predicted by Le Chatelier's principle, enhancing the reaction yield. However, the temperature is optimized to balance reaction efficiency and avoid undesirable side reactions or catalyst deactivation [17].

In the reactor, dehydrogenation occurs to produce acetaldehyde and hydrogen as a by-product. The reactor output is cooled in Cooler 1 and sent to a flash separator to separate acetaldehyde from unreacted ethanol, water, and hydrogen gas. The acetaldehyde-rich stream is further purified in a distillation column. The hydrogen gas is separated by water absorption as a valuable by-product [18]. The use of water (H_2O) as an absorbent in the separation of hydrogen and acetaldehyde is based on the solubility differences between the two compounds in water. Acetaldehyde has significantly higher solubility in water compared to hydrogen, allowing water to effectively absorb acetaldehyde from the gas mixture. Meanwhile, hydrogen, being insoluble in water, remains in the gas phase, enabling efficient separation [19].

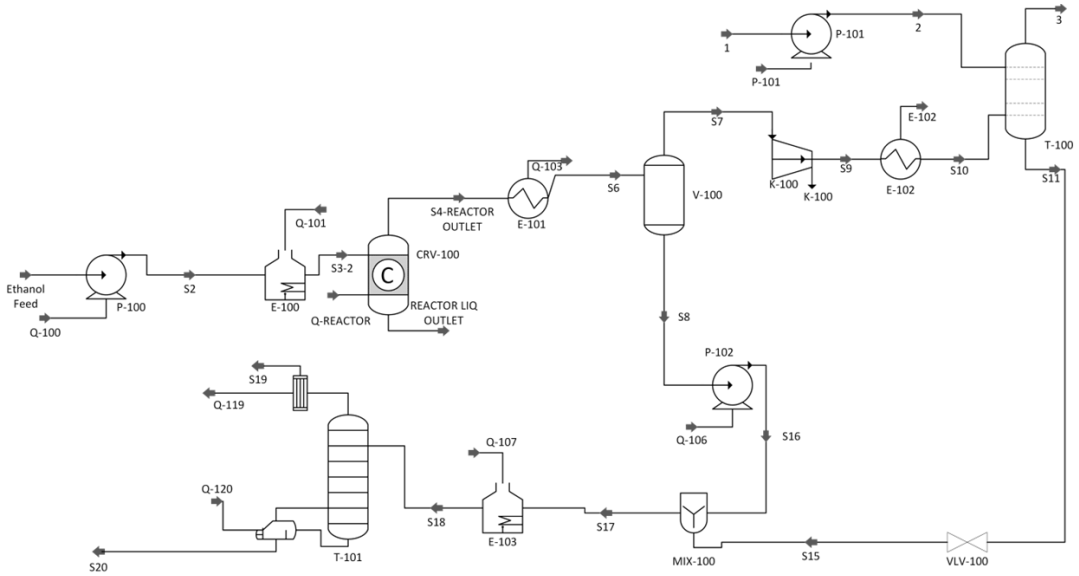

Figure 1. Unmodified process flow diagram to be simulated [20]

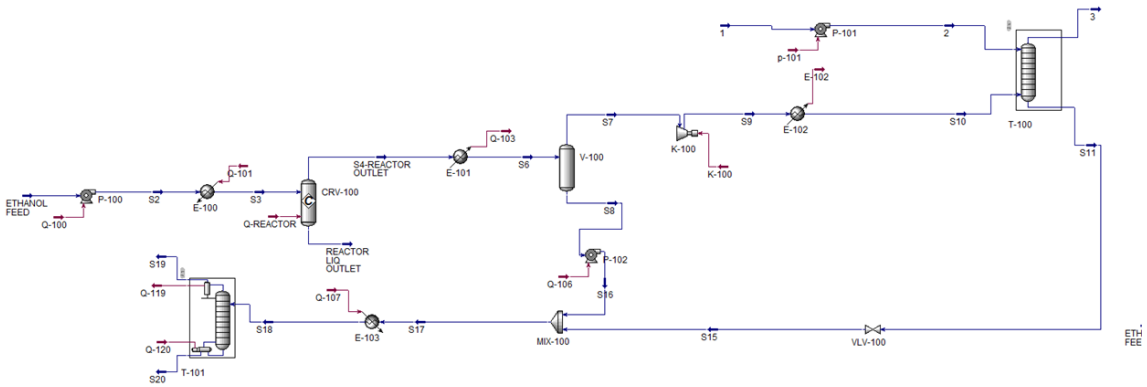

Figure 2. Unmodified/basic process flow diagram from HYSYS simulation

3.2. Thermodynamics Review

The objective of thermodynamic analysis is to determine whether a reaction is exothermic or endothermic and assess its reversibility [21]. Identifying the reaction's thermodynamic nature through enthalpy changes ($\Delta H°_{298K}$) provides critical information for energy management and process optimization. Additionally, evaluating the reversibility of the reaction using Gibbs free energy ($\Delta G°_{298K}$) allows for understanding the reaction's feasibility and equilibrium behavior under given conditions [22]. This analysis is fundamental for designing efficient and sustainable chemical processes, as it informs the selection of operational parameters to maximize yield and minimize energy consumption. The value of $\Delta H_f°$ and $\Delta G_f°$ [23] can be seen in Table 1. The dehydrogenation of ethanol can be expressed as [24] :

$C_2H_5OH \rightarrow CH_3CHO + H_2$

Standard heat of reaction at 298K ($\Delta H°_{298K}$):

$\Delta H°_{298K} = \Sigma\Delta H_f°$ product $- \Sigma\Delta H_f°$ reactant

$\Delta H°_{298K}$ = ($\Delta H_f°$ CH_3CHO + $\Delta H_f°$ H_2) – ($\Delta H_f°$ C_2H_5OH)

$\Delta H°_{298K}$ = ((-166.2) + (0)) – (-235) = 68.8 kJ/mol

Based on the calculations, the result is determined to be positive, indicating that the reaction is endothermic.

Gibbs energy ($\Delta G°_{298K}$):

$\Delta G°_{298K} = \Sigma\Delta G_f°$ product $- \Sigma\Delta G_f°$ reactant

$\Delta G°_{298K}$ = ($\Delta G_f°$ CH_3CHO + $\Delta G_f°$ H_2) – ($\Delta G_f°$ C_2H_5OH)

$\Delta G°_{298K}$ = ((-133) + (0)) – (-167.7) = 33.7 kJ/mol

Equilibrium constant (K_2) in the standard state :

$\Delta G°_{298K} = -RT \ln K$

$$\ln K_2 = -\frac{\Delta G°_{298K}}{RT} = \frac{33.7\frac{kJ}{mol}}{0.008314\frac{kJ}{mol}\times 298\ K} = 13.602$$

$K_2 = 8.0774 \times 10^5$

Equilibrium constant (K_1) at reactor temperature T = 340 °C :

$$ln\frac{K_1}{K_2} = \frac{-\Delta H_R°}{R}\left(\frac{1}{T_2} - \frac{1}{T_1}\right)$$

Where, $\Delta H°_{298K}$ = standard heat of reaction at 25 °C

$$ln\frac{K_1}{8.0774 \times 10^5} = \frac{-68.8\ J/mol}{8.314\frac{J}{mol}.K}\left(\frac{1}{613\ K} - \frac{1}{298\ K}\right)$$

$$ln\frac{K_1}{8.0774 \times 10^5} = 0.0143$$

$$\frac{K_1}{8.0774 \times 10^5} = 1.0144$$

$K_1 = 8.1937 \times 10^{-5}$

Due to the low equilibrium constant, the dehydrogenation of ethanol reaction is reversible.

3.3 Improving Energy Efficiency by adding Heat Exchanger

Based on the simulation results as depicted in Figure 3, information is obtained about the total energy required by the system. This energy is represented in the form of heat flow (kJ/h) generated by the system. This method is used as an approach to illustrate the extent to which energy can be saved when compared to the unmodified system. With this method, we can mathematically calculate the amount of energy saved by the modification process, as well as assess the level of efficiency generated by the process. The heat flow data obtained from the simulation is organized and presented in the form of Table 2 to facilitate analysis.

Table 1. The value of $\Delta H_f°$ and $\Delta G_f°$ of compounds

Compunds	Molecular Formula	$\Delta H_f°$ (kJ/mol)	$\Delta G_f°$ (kJ/mol)
Ethanol	C_2H_5OH	-235	-167.7
Acetaldehyde	CH_3CHO	-166.2	-133
Hydrogen	H_2	0	0

Table 2. Energy of unmodified and modified process

Unmodified Process		Modified Process	
Heat Streams Items	Heat Flow (kJ/h)	Heat Streams Items	Heat Flow (kJ/h)
Q-100	357.8687	Q-100-2	357.8687
Q-101	1,311,097.3855	Q-101-2	309,757.2957
Q-103	1,168,467.3052	Q-103-2	167,127.2154
Q-106	164.7936	Q-106-2	164.7936
Q-107	2,380,943.3893	Q-107-2	2,380,330.2640
Q-119	33,459,461.5065	Q-119-2	33,653,987.7651
Q-120	47,957,443.1439	Q-120-2	48,071,169.3790
K-100	88,000.7335	K-100-3	88,000.7335
E-102	77,150.0577	E-102-3	77,150.0577
p-101	7,262.7175	p-101-3	7,262.7175
Total Heat Flow (kJ/h)	86,450,348.90	Total Heat Flow (kJ/h)	84,755,308.09

In addition, simulation is an important tool in evaluating the performance of a modified system as depicted in Figure 4. By comparing the heat flow data between the modified and unmodified systems, insights can be gained into potential reductions in energy consumption, which can be applied to improvements. The resulting analysis not only shows the direct benefits of energy savings, but also provides guidance for improving sustainability and overall operational efficiency.

$$\Delta H_{Unmodified} = H_{Q-100} + H_{Q-101} + H_{Q-103} + H_{Q-106} + H_{Q-107} + H_{Q-119} + H_{Q-120} + H_{K-100} + H_{E-102} + H_{p-101}$$

$$\Delta H_{Unmodified} = 86{,}450{,}348.90 \text{ kJ/h}$$

$$\Delta H_{Modified} = H_{Q-100-2} + H_{Q-101-2} + H_{Q-103-2} + H_{Q-106-2} + H_{Q-107-2} + H_{Q-119-2} + H_{Q-120-2} + H_{K-100-3} + H_{E-102-3} + H_{p-101-3}$$

$$\Delta H_{Modified} = 84{,}755{,}308.09 \text{ kJ/h}$$

$$Energy\ Reduction = \Delta H_{Unmodified} - \Delta H_{Modified}$$

$$Energy\ Reduction = 86{,}450{,}348.90 \text{ kJ/h} - 84{,}755{,}308.09 \text{kJ/h}$$

$$Energy\ Reduction = 1{,}695{,}040.81 \text{ kJ/h}$$

The increase in energy efficiency is done by adding a heat exchanger (E-104) before the material stream enters the heater (E-100-2), the addition of this heat exchanger is proven to reduce the energy required by the heater to heat the material stream. Before the addition of Heat exchanger (E-104), the heat requirement at Heater (E-100) is 1,311,097.3855 kJ/h on the basic flowsheet, while after the addition of Heat exchanger (E-104) the heat requirement is 309,757.2957 kJ/h on the modified flow sheet, meaning that the heat requirement in the heat exchanger after the addition of Heat Exchanger has decreased by 1,001,304.0898 kJ/h.

3.4 Hydrogen Purity Improvement

The production of acetaldehyde (CH_3CHO) through ethanol dehydrogenation is a significant

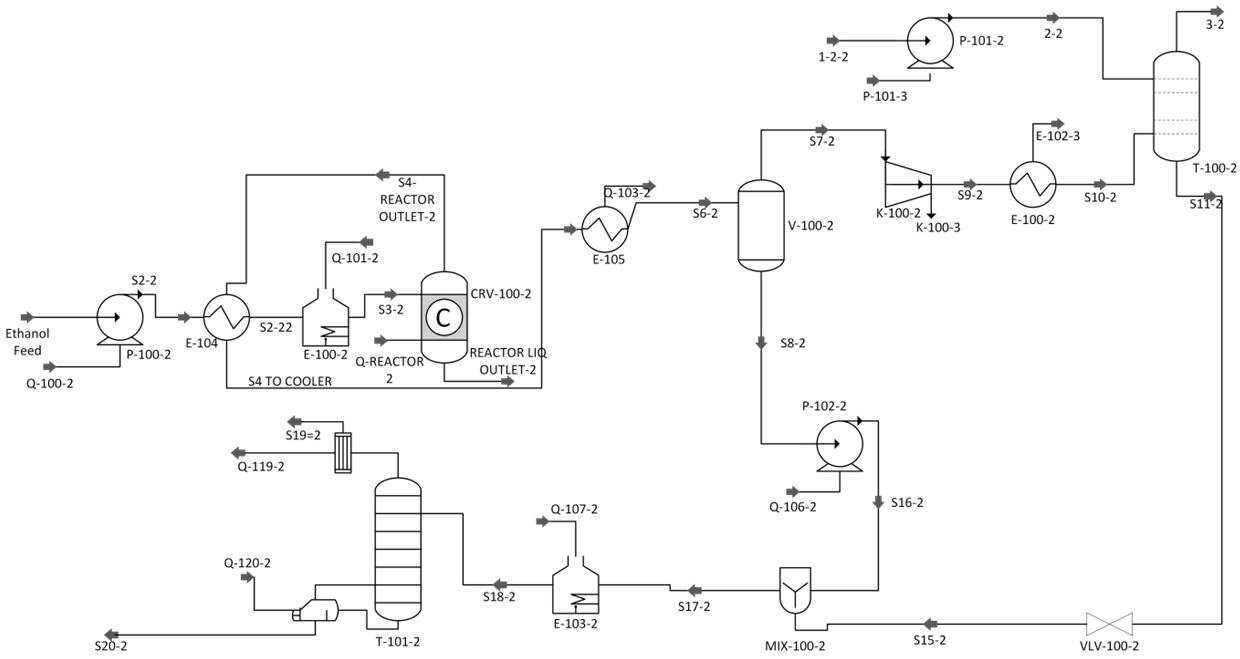

Figure 3. Modified process flow diagram to be simulated.

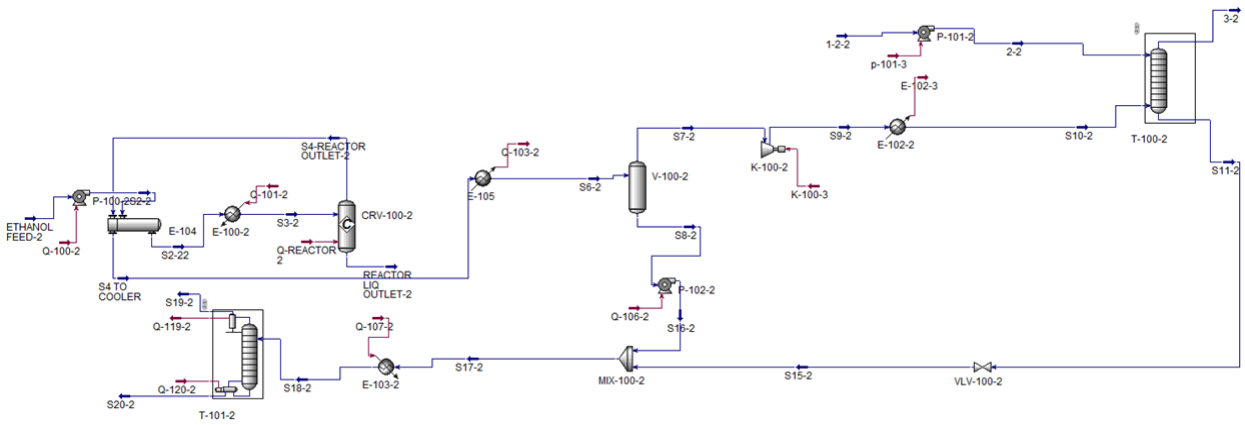

Figure 4. Modified process flow diagram from HYSYS simulation

industrial process that not only produces acetaldehyde but also produces hydrogen as a valuable by-product. Hydrogen purity is essential for its applications, especially in fuel cells and other energy technologies. Increasing hydrogen purity while optimizing energy efficiency in the production process is essential to improve economic sustainability and environmental sustainability. The hydrogen purity can be increased by increasing the mass flow of the absorbent solution [25]. Before modification with a mass flow of water absorbent 6798 kg/hour, a hydrogen purity of 95% was obtained, and when it was modified with a mass flow of water absorbent 10000 kg/hour, a purity of 99.5% was obtained. From the experiments that have been carried out, it can be concluded that the modification can increase the purity of hydrogen by 4.5%.

4. Conclusion

The simulation results demonstrate that the addition of a heat exchanger effectively reduces energy consumption by optimizing heat recovery within the process. The efficiency achieved is proven by the Specific Energy Consumption value of 14,849,129.9774 kJ/ton. Furthermore, the hydrogen purity is significantly improved with an increase in the mass flow of water as an absorbent, enhancing the separation efficiency of hydrogen from acetaldehyde. From the experiments that have been carried out, it can be concluded that the modification can increase the purity of hydrogen by 4.5%. These findings highlight the importance of integrating heat recovery systems and optimizing absorbent flow rates to achieve both energy efficiency and product quality in the process.

CRedit Author Statement

Author Contributions: A. Fawwaz: Conceptualization, Methodology, Investigation, Software, Visualization, Writing, Review & Editing, Supervision; A.P.A. Nugraha: Conceptualization, Methodology, Writing, Review & Editing, Project Administration,Validation; M.P.A Rasyid: Conceptualization, Methodology, Formal Analysis, Resources, Validation, Writing; R.H. Muhammad: Conceptualization, Visualization, Methodology, Investigation, Resources, Data Curation, Writing; .All authors have read and agreed to the published version of the manuscript.

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