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Research Article

Enhancing Energy Efficiency and Ethanol Conversion through the Addition of a Heat Exchanger and Reactor in the Catalytic Dehydration Process for Ethylene Production from Ethanol

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Abstract

Ethylene production requires high energy costs, and the composition of the ethanol feed is not very pure. The aim of this research is to reduce energy costs slightly while still increasing conversion to obtain a purer ethanol conversion. To achieve this goal, the method used is to add one more heat exchanger and one more reactor. The results obtained turned out that by adding a heat exchanger, we do not need cooling water, but can utilize the output of cryogenic distillation. An energy efficiency of 73.56% obtained and the ethanol conversion obtained was also close to pure with the presence of two reactors with a value of 99.2%. Further process creation is needed to be able to optimize the ethylene production process which is more environmentally friendly, such as making ethylene with bioethanol as feed.

Keywords: Energy efficiency; ethanol; ethylene production; optimization

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1. Introduction

Ethylene is a colorless, odorless, and non-toxic gas composed of two carbon atoms and four hydrogen atoms, with the chemical formula C_2H_4 [1]. It is known as an important organic compound, acting as a natural plant hormone and having wide ranging industrial applications. Ethylene has various important applications, especially in agriculture where it is used to stimulate the ripening of fruits and vegetables [2]. It is also a key raw material in the production of various types of plastics, synthetic fibers, and other chemicals [3]. This compound is also utilized as a raw material in chemical synthesis to create various other products such as ethanol, ethylbenzene, and more [4]. As one of the most important organic compounds industrially, ethylene plays a significant role in the global economy and in numerous modern industrial applications [5]. Ethylene stands as a primary petrochemical with a present market valuation of 176 billion USD, projected to reach 287 billion USD by 2030. It serves as a pivotal foundational component for manufacturing polyethylene, polyvinyl chloride, polystyrene, and various copolymers [6]. Additionally, it acts as a key intermediary in producing acetaldehyde, ethylene glycol, ethylene oxide, styrene, ethyl benzene, acetic acid, ethylene dichloride, and vinyl acetate [7].

The demand of ethylene for industrial process in Indonesia is still significantly insufficient. Meeting this demand can be achieved if Indonesia can produce at least 2 million tons of ethylene [8]. It is produced mainly through steam cracking of

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hydrocarbons [9], but alternatively it can be produced through the dehydration of ethanol, which can be produced from a fermentation process using renewable substrates such as glucose, starch, etc. However, in the future indonesia only capable to produced around 400,00 tons of ethylene. The disproportionate demand for ethylene compared its availability has led to substansial import of ethylene. The import of ethylene in 2019 was 706.300,66 tons/year, showing an increase in the import quantity each year since 2017 [10]. It is estimated that the demand for imported ethylene in 2025 will be around 1,024,693.

The reaction employed in the process of producing ethylene is through the dehydration of ethanol, which involves the removal of water molecules from an alcohol compound to yield an alkene compound, commonly referred to as an elimination reaction [11]. Generally, the dehydration reaction of ethanol occurs under endothermic, non-adiabatic, and non isothermal conditions [12]. Production costs and energy costs in producing ethylene are a problem in reaping these benefits [13]. In the process of producing ethylene, it undoubtedly requires energy. The increasing energy demand is closely related to the development of economic activities and uncontrolled population growth. Based on the national energy processing outlook data from 2012 to 2025, the total energy consumption in 2012 reached 1,017 million BTUs, with an annual growth rate between 2012-2025 of 4.5%. According to the national energy usage data in 2013, there are four main sectors accounting for the largest energy consumption: the industry sector at 37.17%, households at 29.43%, transportation at 28.10%, and commercial at 5.28%. And up until now, the majority of energy sources used still come from fossils, namely crude oil at 46.9%, coal at 26.4%, and natural gas at 21.9%. Besides, ethylene production costs depend primarily on the price of ethanol, and currently the price of ethanol is around $910 per ton. High energy costs also account for a large portion of production costs [14].

In previous research, for energy costs, lowering the reaction temperature while still achieving high selectivity was a priority, but the exit fluid can also be used as a heating fluid to recover heat and save energy. Analysis of heat recovery and conservation that has the potential to reduce these costs [15]. Different ethanol feedstock sources contain different impurities, which may affect the catalytic ability or lifetime of a particular catalyst in different ways [16]. Thus, the aim of this research is to reduce energy costs slightly while still increasing conversion in order to obtain a purer ethanol conversion

2. Methods

2.1. Feed Preparation

The main raw material used in this process is ethanol. As depicted in Figure 1, initially, ethanol is stored in the raw material tanks, then it is transferred to the vaporizer. Subsequently, the resulting products from the vaporizer, in the form of vapor and liquid phases, enter the separator to be separated according to their phases. The output from the top of the separator is in the gas phase, while the output from the bottom is in the liquid phase, which is recycled back into the vaporizer. The ethanol in the gas phase enters the heat exchanger to raise its temperature.

2.2. Catalytic Dehydration of Ethanol to Ethylene

Catalytic dehydration of ethanol is an alternative route for production of ethylene. The first report on catalytic dehydration of ethanol to ethylene was published in the literature in 1797. However, the first commercial plant was started in the beginning of the 20th century. In the industry, the alcohol dehydration mainly occurs in the vapor phase of two-catalyst systems, i.e., supported phosphoric acid and activated alumina. Most old technologies used phosphoric acid while the activated alumina became predominant later. The ethanol dehydration is an endothermic reaction (requiring 1632 J.g^{-1} or 390 cal.g^{-1} of ethylene formed). Therefore, the reaction temperature affects the yield of ethylene. The highest selectivity towards ethylene is obtained at 300–500 ^{o}C (Eq. (1)). Higher temperatures shift the reaction towards acetaldehyde production (Eq. (2)), while lower temperatures result in production of diethyl ether (Eq. (3)). Isothermal and adiabatic modes of operations have been suggested for the dehydration of ethanol to ethylene, while the latter is more economically feasible [4]. The dehydration reaction of ethanol produces products in the form of ethylene and water. In this process, high temperatures are

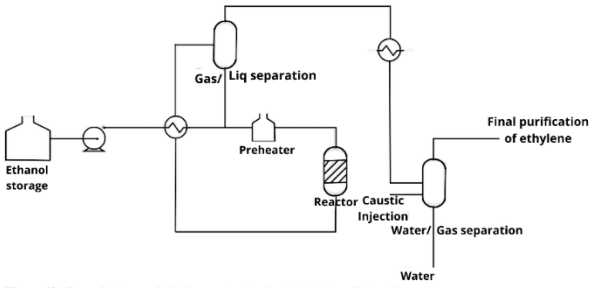

Figure 1. General scheme of ethylene production by dehydration of ethanol [17]

used, specifically 750 °F, because it is expected that the reaction predominantly leads to the production of the product and yield ethylene with high conversion. Processes operating under these conditions typically yield by-products, therefore separation is required to obtain ethylene with high purity.

Main reaction:

$$C_2H_5OH \rightarrow C_2H_4 + H_2 \quad (1)$$

Side reactions:

$$C_2H_5OH \rightarrow (C_2H_5)_2O + H_2O \quad (2)$$

$$C_2H_5OH \rightarrow C_2H_4O + H_2 \quad (3)$$

Ethanol conversion can be calculated as follow:

$$\text{Ethanol Conversion} = \frac{\text{Reacted Ethanol}}{\text{Ethanol Input}} \times 100\% \quad (4)$$

Energy loss efficiency can be calculated as follow:

$$\text{Energy loss efficiency} = 1 - \frac{\text{After modification}}{\text{Before modification}} \times 100\% \quad (5)$$

2.3. Process Modification

By utilizing ASPEN HYSYS application, the catalytic dehydration process of ethanol to ethylene is simulated and the process modification is carried out in the form of the addition of a heat exchanger. The addition of a heat exchanger was carried out to reduce the energy requirements previously used to heat cooling water. Apart from that, the cryogenic distillation method plays a role in separation which aims to obtain a low temperature product, so that it does not require a cooler again. The output from cryogenic distillation is reused to then enter the heat exchanger. This causes the process energy efficiency value to be higher than before the process modification. Apart from that, if one reactor is used in a simple scheme, it turns out that the ethanol purity is still lacking. Therefore, two reactors were used to obtain purer ethanol purity.

To assess whether the modified process is better, several benchmarks and parameters can be used. Here are some key parameters and methods to evaluate them:

(a) Energy Efficiency: Parameter: total energy usage before and after modification. Calculation Method: comparing the amount of energy used for heating and cooling the process before and after modification. Energy efficiency can be calculated using the following equation:

$$\text{Energy efficiency} = \frac{\text{Energy saved}}{\text{Total energy used}} \times 100\% \quad (6)$$

For example, if the total energy used before modification is E_{before} and after modification is E_{after}, the Energy Efficiency Improvement can be calculated:

$$\text{Energy Efficiency Improvement} = \frac{\text{Energy before} - \text{Energy after}}{\text{Energy before}} \times 100\% \quad (7)$$

(b) Conversion and Selectivity: parameter: percentage of ethanol conversion and selectivity towards ethylene. Calculation method: ethanol conversion can be calculated using Equation (4), while ethylene selectivity can be calculated as follow:

$$\text{Selectivity} = \frac{\text{Amount of ethylene produced}}{\text{Total products}} \times 100\% \quad (8)$$

(c) Product Purity: Parameter: purity of ethylene and ethanol in the product stream. Calculation Method: by analyzing the composition of the product stream using tools like Gas Chromatography (GC) or data output from the HYSYS simulation and comparing the product purity before and after modification.

3. Results and Discussion

3.1. Operating Conditions

The reactor pressure used in the catalytic dehydration process of ethanol to ethylene is 40 atm. This pressure was chosen because the dehydration reaction can occur at a pressure of 40-45 atm. The temperature used in the catalytic dehydration process of ethanol to ethylene is 500 °C This temperature was chosen because the catalyst used in this process, namely sulfuric acid, requires a temperature in the range of 400 °C - 500 °C, so it is hoped that at this temperature the reaction easily run in the right direction and produces ethylene products with high conversion.

The reactor used in the catalytic dehydration process of ethanol to ethylene is an adiabatic reactor, where the reactor operates without any heat exchange with the environment, so steam is used as a heater. Using a heater can reduce the amount of catalyst needed and reduce the formation of by-products, thereby increasing investment costs for ethylene products. The reaction phase in the catalytic dehydration process of ethanol to ethylene is the liquid phase, because in the literature the catalyst used is a homogeneous catalyst, namely sulfuric acid, where the sulfuric acid is in the liquid phase. So it can be ascertained that the reaction phase is the liquid phase.

3.2. Thermodynamics Aspect

In the simulation, the reaction is carried out at a temperature of 500 °C or 773 K. ΔH reaction at 773 K is found using the following equations and Table 1:

$$\Delta H°_{reaction,\ 298K} = \Delta H°_{f,\ product} - \Delta H°_{f,\ reactant} \quad (1)$$

$$\Delta H°_{773} = \Delta H°_{298} + \int_{298}^{773} Cp\ dT \quad (2)$$

$$\Delta H°_{773} = \Delta H°_{298} + \int_{298}^{773} A + BT + CT^2 + DT^3 + ET^4\ dT \quad (3)$$

Based on Equations (2) and (3) and Table 1, $\Delta H°_{773K,ethanol}$ = -188511.32 J/mol, $\Delta H°_{773K,water}$ = -2248356.37 J/mol, and $\Delta H°_{773K,ethylene}$ = 82715.99 J/mol. Therefore, $\Delta H°_{773K,reaction}$ = 46390.93 J/mol

The reaction enthalpy data is known to be positive, so the reaction takes place endothermically. The Gibbs free energy of reaction at a temperature of 773K (7800 J/mol) can be found using the following equation:

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

3.3. Basic and Modified Process Flow Diagram (PFD)

Basic and Modified Process Flow Diagram are depicted in Figures (2)-(5). The catalytic dehydration process of ethanol to ethylene use two reactors. This aims to increase ethanol conversion. When using one reactor, only a conversion of 90.97% is obtained. Therefore, three

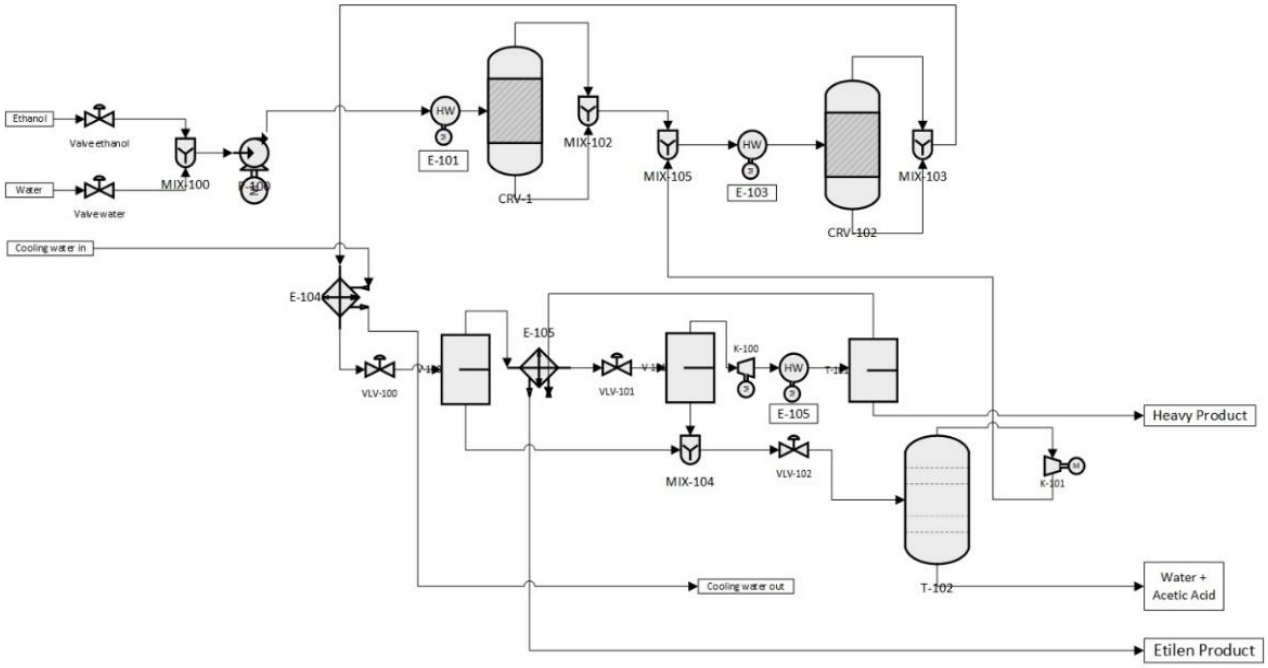

Figure 2. Basic Process Flow Diagram (PFD) before modification process

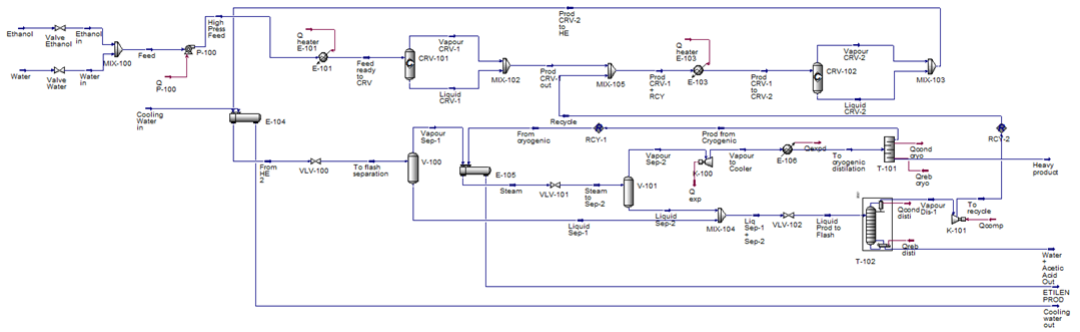

Figure 3. Process flow diagram before modification process using Aspen Hysys V12

Table 2. Data of enthalpy and Gibbs free energy formation of ethanol, water, ethylene [17]

Compound	$\Delta H°_{f,298}$ (J/mol)	A	B	C	D	E	$\Delta G°_{f,298K}$ (J/mol)
Ethanol	-234.810	27.091	1.1055×10^{-1}	1.0957×10^{-4}	-1.5046×10^{-7}	4.6601×10^{-11}	-168.28
Water	-241.800	33.933	-8.4186×10^{-3}	2.9906×10^{-5}	-1.7825×10^{-8}	3.6934×10^{-12}	-228.60
Ethylene	52.300	32.083	-1.4831×10^{-2}	2.4774×10^{-4}	-2.3766×10^{-7}	6.8274×10^{-11}	68.12

reactors were used with the resulting conversion being 9%. This can be known through the following calculations. Ethanol in Feed is 0.9034 weight fraction, while weight fraction of ethanol in product stream (CRV-1 and CRV-2) is 0.0484 and 0.0072, respectively. If only one reactor is used, the conversion calculation is obtained as Ethanol Conversion = 94.64%, while if two reactors are used, the conversion calculation is obtained as Ethanol Conversion = 99.2%. Therefore, it was found that with two reactors the purity of the ethanol feed became higher.

Before modification, cooling water is used in the heat exchanger. After modification, the cooling water is replaced using another heat exchanger before entering another heat exchanger. The added heat exchanger uses the output from the second reactor. Comparation of energy heater before and after modification are 488,991,768.98 kJ/h and129,263,686.96 kJ/h, respectively. Therefore, energy loss efficiency is 73.56 %. Thus, it is found that with two heat exchangers we can save energy with an efficiency of 73.56%.

4. Conclusion

The results obtained turned out that by adding a heat exchanger, we do not need cooling water, but can utilize the output of cryogenic distillation. An energy loss efficiency of 73.56% was obtained and the ethanol conversion obtained was also close to pure with the presence of two reactors with a value of 99.2%. Further process creation is needed to be able to optimize the ethylene production process and be more environmentally friendly, for example making ethylene with bioethanol as feed.

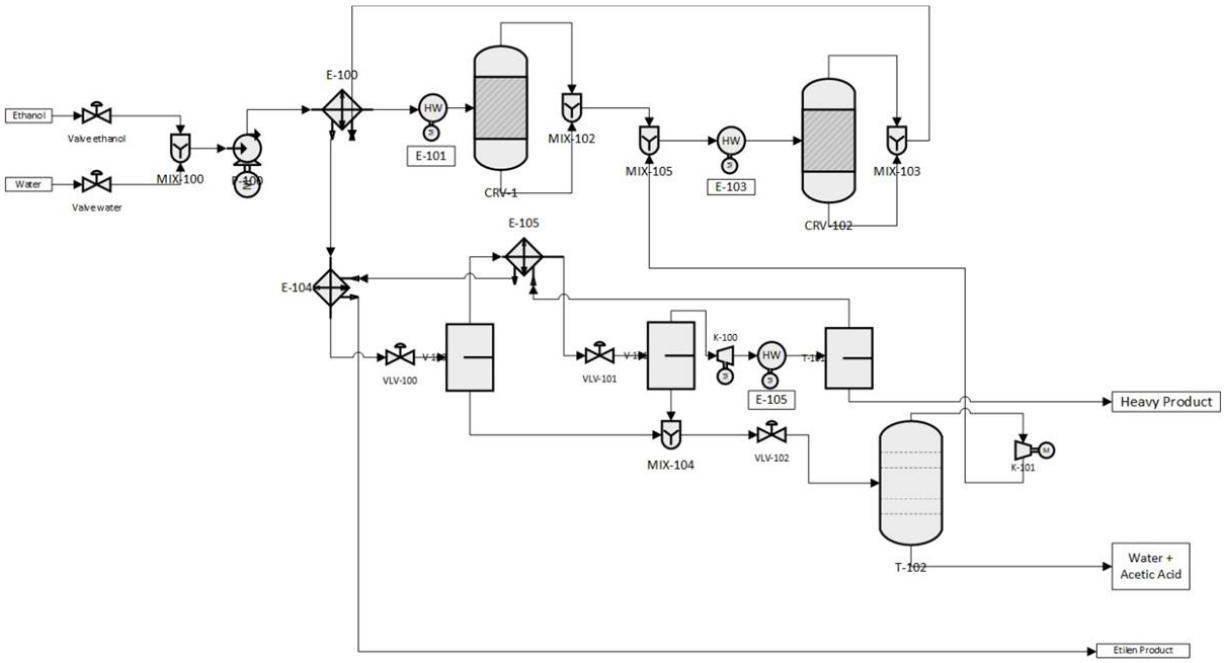

Figure 4. Modified Process Flow Diagram (PFD) after modification process

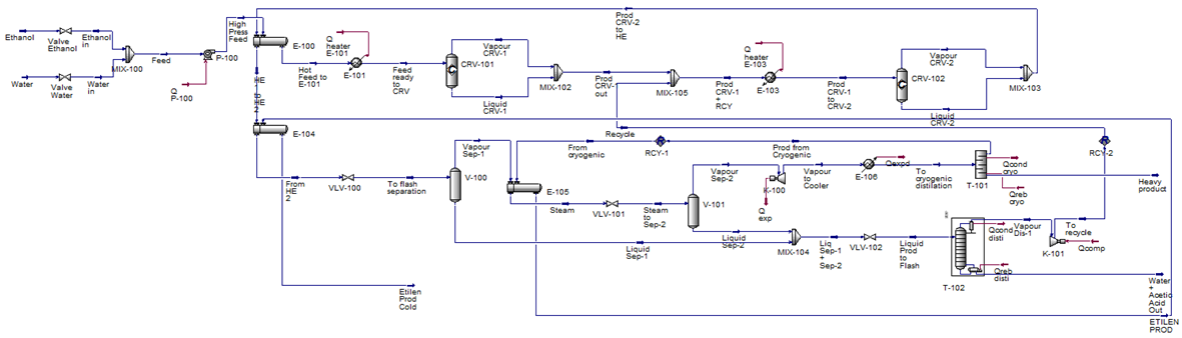

Figure 5. Simulation of Modified Process Flow Diagram using Aspen Hysys V12

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