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Research Article

Integration of Heat Exchangers, Compressor, and Steam Reutilization for Energy Efficiency Improvement in Thermal Systems of Dimethyl Ether (DME) Production

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Abstract

Dimethyl ether (DME) is widely recommended as an environmentally friendly aerosol and green refrigerant due to its low ozone depletion potential and lower global warming potential. Dimethyl ether is produced through the dehydration of methanol which has the potential to be an environmentally friendly alternative fuel. This research addresses the improvement of energy efficiency in dimethyl ether (DME) production through the modification of a heat transfer unit using Aspen HYSYS process simulation software. Dimethyl ether is an environmentally friendly chemical with low global warming potential, which is produced through methanol dehydration. This study focuses on the replacement of heaters and coolers. These modifications successfully improved energy efficiency by reducing net energy consumption from 4.867E+6 kJ/h to 3.268E+5 kJ/h. Despite the decrease in energy efficiency, the conversion rate remained the same at 99.7%. This research shows that modification of the heat transfer system can support more energy-efficient and sustainable DME production.

Keywords: Energy; Dimethyl Ether; Advanced; Heat Transfer; Aspen HYSYS; DME

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1. Introduction

Dimethyl ether (DME) is widely recommended as an environmentally friendly aerosol and green refrigerant due to its low ozone depletion potential and lower global warming potential [1]. DME can be produced from a wide variety of feedstocks including natural gas, crude oil, residual oils, coal, and waste products. Beyond several raw materials, natural gas is the most promising raw material because of its wide availability [2].

Dimethyl ether (DME) can be synthesized using two primary methods: (1) the one-stage direct process and (2) the two-stage indirect process [3]. In the one-stage process, DME is produced directly from syngas. Conversely, in the two-stage method, syngas is initially converted into methanol, which is then used to produce DME [4].

Based on previous research [5], the design of a DME synthesis plant has been made with the use of a heater for pre-heating treatment which will be increased in temperature using a heat exchanger with a steam temperature of 525 °F. After leaving the reactor, the product is cooled with a cooler to a temperature of 84 °C. The use of

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this method has a disadvantage in production costs, which requires a large amount of energy. Therefore, an energy saving innovation is made by replacing the use of a heater with a heat exchanger which is then compressed with a compressor to help increase the temperature to the desired temperature. HE-1 output steam can be used to cool the product temperature as an innovation to replace the cooler with a heat exchanger as well. This paper aims to examine the effect of replacing the use of heater and cooler with heat exchanger and utilize the heat exchanger output steam for the next process in minimizing energy requirements which has never been done in previous research studies.

To improve DME production from both economic and operational standpoints, there is a need to design a dimethyl ether plant using simulations that incorporate heat transfer considerations. Research suggests that this challenge can be addressed by applying sustainable design practices throughout various process stages. Optimizing energy efficiency is essential for meeting critical objectives in the industrial sector.

2. Methods

2.1 Process Simulators using HYSYS

The use of process simulation software has had a great impact on the chemical engineering (ChE) curricula during the last few years, being a very powerful tool for the design and operation of chemical plants [6]. One of the most popular commercial process simulators is Aspen HYSYS. Aspen HYSYS is a process simulator widely used at the industrial level, especially for performing conceptual design, control, optimization and monitoring of processes at various stages of any project [7].

Process simulator is defined as an engineering tool which performs automated calculations, mass and energy balances, physical property estimations, design or rating calculations, costing, process optimization, accurate description of physical properties of pure components and complex mixture, models for a large variety of reactors and unit operations, numerical techniques for solving large systems of algebraic and differential equations [8]. In this work Aspen HYSYS V11 was used to simulate production of DME. Some of its capabilities include highly interactive process flow diagrams for building and navigating through large simulations [9]. The program also provides highly flexible and easy-to-use modeling of unit operations, such as distillation, reactors, heat transfer operations, rotating equipment, controllers, and logical operations in both steady-state and dynamic environments. In addition, ASPEN HYSYS provides comprehensive thermodynamics for accurate calculations of physical properties, transport properties, and phase behavior [10].

2.2 Methanol Dehydration

The process of compound dehydration refers to the chemical reaction in which a compound loses water molecules, leading to the formation of new compounds [11]. Methanol dehydration is a crucial chemical process used primarily for the production of dimethyl ether (DME), a valuable fuel and chemical feedstock. The reaction typically involves converting methanol (CH_3OH) into DME (CH_3OCH_3) through catalytic dehydration [12]. This process can be optimized in various ways to improve efficiency and reduce energy consumption. The dehydration of methanol can be represented by the following reaction:

$$2CH_3OH \rightarrow CH_3OCH_3 + H_2O \quad (1)$$

This reaction is exothermic and the higher the temperature, the lower the conversion [13]. This reaction proceeds without any change in the number of moles and is unaffected by reaction pressure in terms of thermodynamics, but its thermodynamic favorability increases at lower temperatures. This reaction is generally facilitated by acidic catalysts, such as alumina (Al_2O_3), zeolites, or silica-alumina, which help in breaking the O-H bonds in methanol and facilitating the formation of DME and water as by-products [14]. The reaction typically occurs at elevated temperatures (200 – 400 °C) and moderate pressures (10 – 20 bar) to optimize conversion rates and selectivity towards DME [15].

2.3 Basic Process Flow Diagram from Literatures

Turton [5] in their book have designed a dimethyl ether (DME) plant simulation with methanol as raw material. The plant is designed with a capacity of 15,000 tons/year. The vapor phase properties are calculated from the Peng-Robinson equation of state. The Peng-Robinson (PR) equation of state is a modification of the Redlich-Kwong equation of state and was published by Peng and Robinson in 1976. Only critical data of pure substances are a prerequisite for application due to the simple pattern and common parameters for the PR equation[16]. Based on Figure 1, the dimethyl ether synthesis process begins by mixing pure methanol with recycled methanol. After that, the pressure will be increased to 9 atm using a pump and the pre-heating process is carried out to 180 °C. The saturated steam is reheated to 250 °C using a heat exchanger which then enters a plug flow reactor.

Equation (1) is used as the kinetic equation in the dimethyl ether formation process.

$$-r = 1.21 \times 10^{-1} \times e^{\left(\frac{80.480}{RT}\right)} \quad (2)$$

The conversion obtained in the reactor is 99.7%. Then the pressure is reduced using a valve to 8 atm and cooled using a cooler to 148 °C. Furthermore, dimethyl ether was separated from water and methanol using a distillation column and obtained a purity of 99.9% dimethyl ether. The bottom result is cooled again to 84 °C so that the mixture is in its saturated liquid phase. Methanol is then separated from water by distillation and the remaining methanol is recycled to feed for reuse.

2.4 Strategy Modification Heat Transfer Unit

The use of heat exchangers is based on the principles of thermodynamics and heat transfer [17]. The use of heat exchangers can be used to optimize the performance of heat exchanger itself, reduce waste energy, and improve operational efficiency [18]. The heating process in a heat exchanger is essentially about transferring heat energy from one fluid to another without mixing them. This concept is very important in various industrial applications where maintaining a certain temperature is crucial for efficiency and effectiveness. Thus, heat exchangers do not inherently require external energy for heating [19].

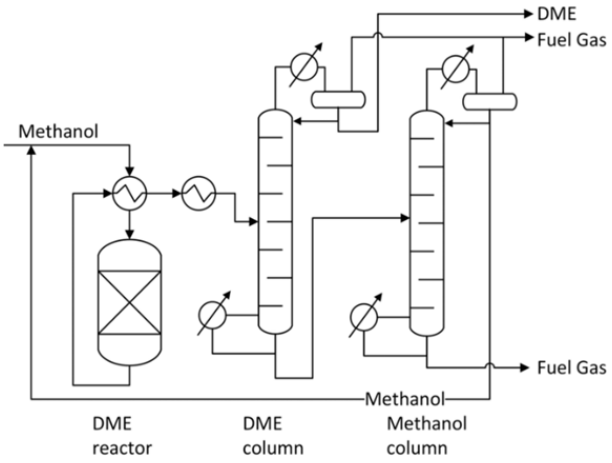

Figure 1. Basic process flow diagram [2]

Heaters generally require an external energy source to generate heat, which depends on their type and design [20]. This heating process involves the conversion of electrical energy into heat, which is mainly based on the Joule heating principle[21]. Joule heating, or resistive heating, is a process in which electrical energy is converted into heat through the resistance of a conductor when an electric current flows through it [22]. This phenomenon occurs when an electric current passes through a resistive material, which generates heat. The relationship between current, resistance, and time can be explained by Joule's law [23].

$$Q = I^2 \times R \quad (3)$$

The same thing as a heater, a cooler also requires electrical energy to lower the temperature [24]. In the other hand, the use of a compressor after the heat exchanger is able to increase the pressure and the temperature increases. It is according to the ideal gas law.

$$PV = nRT \quad (4)$$

When the pressure increases during compression, the temperature also increases [25].

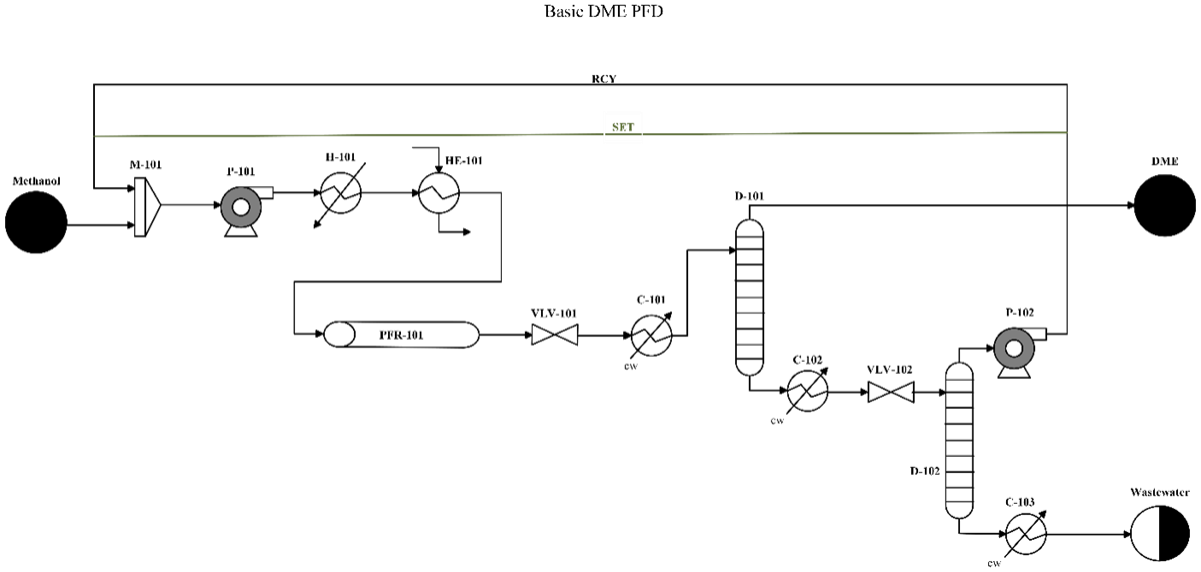

Figure 2. Process Flow Diagram (PFD) of basic process after process creation

In this study, an innovation was developed in the form of using a heat exchanger to replace the heater in the pre-heating process. In addition, a compressor is also used to increase the gas pressure and temperature to operating temperature. The heat exchanger output steam is used to cool the reactor product using a heat exchanger instead of a cooler. Thus, energy usage can be reduced.

3. Results and Discussion

3.1 Basic PFD and Modification to Enhancing Energi Efficiency

The design capacity of an industrial DME production plant is 15,000 metric tons of DME per year. In this study, the Peng-Robinson Stryjek-Vera (PRSV) equation of state is used to review the thermodynamic properties. The dehydration reaction shown in Equation (1) is carried out in a fixed bed reactor. Figure 2 is the flow sheet diagrams of the basic DME plant design. The feed, namely Methanol, is fed into the system at a temperature of 30 ℃, 77.61 kgmole/h, and 1.03 bar from the methanol synthesis plant and mixed with the recycle from stream R-001. Then the pressure is increased to 15.20 bar by using a pump. This mixture is preheated in a heat exchanger (HE) and evaporated in a heater before entering the reactor. After entering the reactor, the components in the stream will consist of DME, CH_3OH, and H_2O. The reactor outlet stream will be used in a heat exchanger (HE) and cooled in a cooler, partially decompressed, and fed into a distillation tower. DME is obtained in column D-001 with a high purity of 96.41% which is then sent to the processing section. Furthermore, in column D-002, water and methanol are separated. The final result, water sent to cooler C-003 to lower the temperature, while methanol will be recycled to be reused as a feed mixture.

Figure 4 depicts the PFD of modified process, while the mass energy balance is presented in Table S2 (Supporting Information). Modifications are made by replacing the heater with a heat exchanger where this aims to improve energy efficiency. Also, after the heat exchanger was added, a compressor was introduced before the reactor to increase the feed pressure. Since the compressor has a side effect of increasing the temperature, this effect can be utilized to increase the feed temperature to the reaction temperature. Then the chemical reaction in the CRV-100 reactor is exothermic, which ultimately generates heat. The reactor output product is then cooled

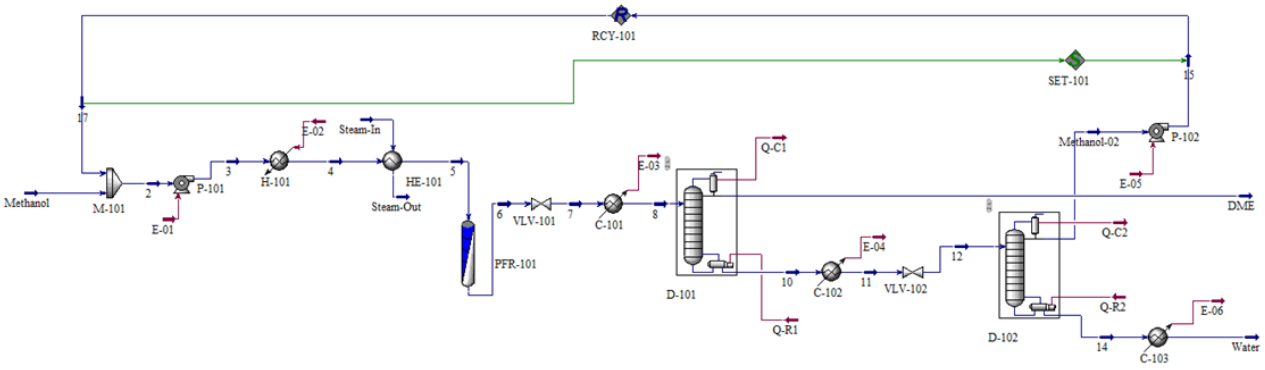

Figure 3. Aspen HYSYS simulation of basic process before process creation

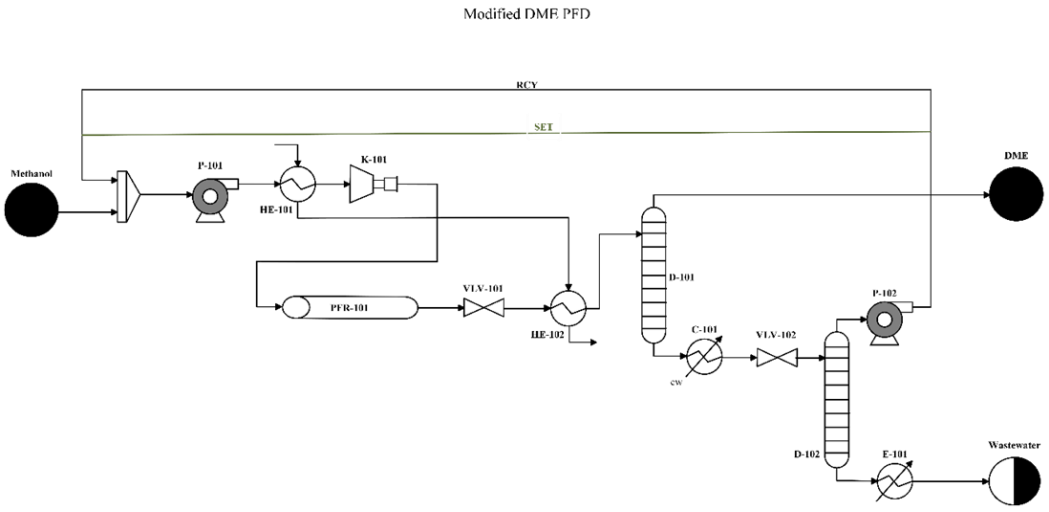

Figure 4. Process Flow Diagram (PFD) of modified process after process creation

using the heat exchanger output steam (HE-01). After modification, the net energy reduction obtained reached 3.268E5 kJ/h.

3.2 Thermodynamics and Operating Conditions Consideration

Thermodynamic calculations and experiments complement each other: calculations facilitate a more comprehensive interpretation of limited experimental data and help in identifying critical experiments to apply, while experiments supply the data required to validate calculation results and offer input parameters for modeling [26]. Thermodynamic calculation also needed to improve the direction of reactions, i.e. reversible / irreversible [27]. In the selected process, one reactor is used and methanol dehydration process occur.

3.2.1 Heat of reaction ΔH^{o}_{298K}

The main reaction from Equation (1) has the value $\Delta H^{o}_{f,298K}$ of each component and $\Delta H^{o}_{r,298K}$ at a temperature of 298 K. Table 1. obtains the data of each value of $\Delta H^{o}_{f,298K}$ and it can be seen as follow [28]:

$2CH_3OH_{(g)} \rightarrow (CH_3)_2O_{(g)} + H_2O_{(g)}$

$\Delta H^{o}_{r,298K} = \sum \Delta H^{o}_{f,298K,product} - \Delta H^{o}_{f,298K,\ reactant}$

$\Delta H^{o}_{r,298K} = \Delta H^{o}_{f,298K,\ (CH_3)_2O} + \Delta H^{o}_{f,298K,\ H_2O} - 2\Delta H^{o}_{f,298K,\ CH_3OH}$

$\Delta H^{o}_{r,298K} = (-184.1 + (-241.8)) - (2 \times (-201.17))$ kJ/mol

$\Delta H^{o}_{r,298K} = -23.56$ kJ/mol

Table 1. Enthalpy information of the main reaction

Compounds	Molecular Formula	$\Delta H^{o}_{f,298K}$ (kJ/mol)
Methanol	CH_3OH	-201.17
Dimethyl Ether	$(CH_3)_2O$	-184.1
Water	H_2O	-241.8

Based on the above calculations, we obtain the value of $\Delta H^{o}_{r,298K} = -23.56$ kJ/mol. We can conclude the reaction is exothermic or a reaction that produces heat due to its negative value (-).

3.2.2 Gibbs Free Energy

The value $\Delta G^{o}_{f,298K}$ of each component at a temperature of 298 K can be seen in Table 2. Based on the data in Table 2, the $\Delta G^{o}_{r,298K}$ of dehydrogenation reaction is as follows [28]:

$\Delta G^{o}_{r,298K} = \sum \Delta G^{o}_{f,298K,product} - \Delta G^{o}_{f,298K,\ reactant}$

$\Delta G^{o}_{r,298K} = \Delta G^{o}_{f,298K,\ (CH_3)_2O} + \Delta G^{o}_{f,298K,\ H_2O} - 2\Delta G^{o}_{f,298K,\ CH_3OH}$

$\Delta G^{o}_{r,298K} = (-112.9 + (-228.6)) - (2 \times (-162.51))$ kJ/mol

$\Delta G^{o}_{r,298K} = -16.48$ kJ/mol

From the above calculation, we obtain the value of $\Delta G^{o}_{r,298K} = -16.48$ kJ/mol. This reaction takes place spontaneously due to its result from the calculation of $\Delta G^{o}_{r,298K} < 0$. Operation takes place of temperature at 250-400 °C. The calculation value of K_{298}, $K_{523.15}$, and $K_{673.15}$ to determine the magnitude of the equilibrium constant (K) can be seen as follows [28]:

$$\ln K_{298} = \frac{-\Delta G}{R.T}$$

$$\ln K_{298} = \frac{-(-16{,}480\ \text{J/mol})}{8.314\ \text{J/mol.K} \times 298\ \text{K}}$$

$K_{298} = 774.079$

Value of $K_{523.15}$:

$$\ln \frac{K_{523.15}}{K_{298}} = -\frac{\Delta H^{o}_{298K}}{R} \times \left(\frac{1}{T_{523.15}} - \frac{1}{T_{298}}\right)$$

Table 2. Gibbs' free energy information of the main reaction

Compounds	Molecular Formula	$\Delta G^{o}_{f,298K}$ (kJ/mol)
Methanol	CH_3OH	-162.51
Dimethyl Ether	$(CH_3)_2O$	-112.9
Water	H_2O	-228.6

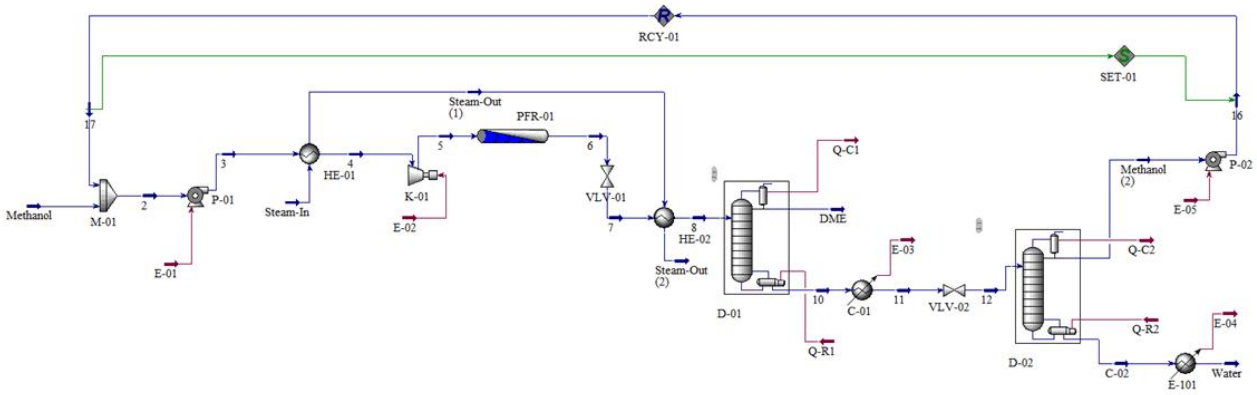

Figure 5. Aspen HYSYS simulation of modified process after process

$$\ln\frac{K_{523.15}}{774.079} = -\frac{-23{,}560\ \text{J/mol}}{8.314\ \text{J/mol.K}} \times \left(\frac{1}{523.15\ \text{K}} - \frac{1}{298\ \text{K}}\right)$$

$$\ln\frac{K_{523.15}}{774.079} = -4.093$$

Thus, $K_{523.15} = 12.919$

Value of $K_{673.15}$:

$$\ln\frac{K_{673.15}}{K_{298}} = -\frac{\Delta H^{o}_{298K}}{R} \times \left(\frac{1}{T_{673.15}} - \frac{1}{T_{298}}\right)$$

$$\ln\frac{K_{673.15}}{774.079} = -\frac{-23{,}560\ \text{J/mol}}{8.314\ \text{J/mol.K}} \times \left(\frac{1}{673.15\text{K}} - \frac{1}{298\ \text{K}}\right)$$

$$\ln\frac{K_{673.15}}{774.079} = -5.300$$

Thus, $K_{673.15} = 3.864$

The equilibrium constants of the reaction at temperatures of 250 °C and 400 °C are 12.919 and 3.864, respectively. This indicates that under both conditions, the reaction proceeds irreversibly.

3.3 Optimize Energy Efficiency by Process Modification

In this study, a modification of the heat transfer unit was carried out in the methanol dehydration process for DME production. In Figure 3, the basic plant design uses a heater which requires higher energy. Modifications were made by replacing the heat transfer unit, namely replacing one heating unit with a heat exchanger (HE) unit and then adding a compressor after the heat exchanger. Additionally, the modification involves replacing the cooler with heat exchanger and repurposing steam from the first heat exchanger to be directed to the second one. This modification results in a reduction of energy consumption so that it can later suppress or reduce production costs. This modification is also displayed in the form of an Aspen HYSYS flow diagram as shown in Figure 5. Based on Table 3, the net energy generated by the heating equipment in the production process is 4.867E6 kJ/h. Then, Table 4 shows the amount of energy required by the heating device in the process after modification with a total energy of 3.268E5 kJ/h. This indicates an energy efficiency improvement of 93.3%. Table S1 (Supporting Information) presents the energy stream of modified process.

The decrease in energy that occurs is due to the replacement of equipment from heaters and coolers with heat exchangers and compressors. Heater and cooler require external energy to increase and decrease the temperature of the material [20]. While the concept of using a heat exchanger is to exchange heat between 2 different materials. The hot steam previously used to heat the feed turns cold and can be used to cool the reactor product whose temperature is hotter. With the concept of exchange, no external energy is required to assist the process of lowering or increasing the temperature [19]. The use of the compressor itself in addition to increasing pressure, has the effect of increasing the temperature of the material [25]. So that its use can be useful for reducing energy.

Table 3. Net energy of basic plant

Properties	Duty (kJ/h)
P-101	6,075.887
H-101	3.564e+006
HE-101	3.219e+005
	-3.219e+005
C-101	1.297e+006
Total	4.867e+006

Tabel 4. Net energy of modified plant.

Properties	Duty (kJ/h)
P-101	2,568.956
HE-101	3.565e+006
	-3.565e+006
K-101	3.242e+005
HE-102	1.143e+006
	-1.143e+006
Total	3.268e+005

4. Conclusion

Based on this study, DME plant simulation using Aspen HYSYS process simulator is able to produce high purity DME (15,000 tons per year) from methanol. The simulated net energy can be reduced from 4.867E6 kJ/h to 3.268E5 kJ/h by changing the heater with a heat exchanger where this aims to increase energy efficiency, and adding a compressor afterwards where this aims to increase the feed pressure and temperature and it can be utilized to increase the feed temperature to the reaction temperature. So, it can be concluded that DME production from methanol dehydration successfully increased energy efficiency by reducing net energy consumption with improvement of 93.3%.

CRediT Author Statement

Authors Contribution: F. Wijaya: Conceptualization, Formal Analysis, Investigation, Software, Visualization, Writing, Review & Editing, Supervision; G.F. Putri: Conceptualization, Methodology, Visualization, Writing, Software, Review & Editing, Project Administration, Validation; C.P. Sukmajati:

Table 5. Comparison of the net energy of basic and modified

Net Energy Before Modified (kJ/h)	Net Energy After Modified (kJ/h)
4.867e+006	3.268e+005

Conceptualization, Methodology, Resources, Validation, Writing; A.M. Dewi: Formal Analysis, Methodology, Investigation, Resources, Data Curation, Writing; W.M.N. Asyhari: Formal Analysis, Writing. All authors have read and agreed to the published version of the manuscript.

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