

Reducing Energy Consumption in the Synthesis of Dimethyl Ether (DME) from Methanol Dehydration by Modifying Heat Transfer Unit Using Aspen HYSYS

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Abstract

In the pursuit of a transport sector free from fossil fuels, the incorporation of Dimethyl ether (DME) emerges as a commendable ecological substitute. The DME is a synthetically produced serves as a viable alternative to conventional fuels such as diesel and liquified petroleum gas (LPG). The Dimethyl Ether (DME) production is carried out by catalytic dehydration of methanol over an acidic zeolite-based catalyst. The technological process for the DME synthesis was simulated using Aspen HYSYS based on the combined operating parameters of the reaction dynamic model for the methanol dehydration reaction. This paper attempts to evaluate a modification in dehydration of methanol process to reducing energy consumption by modifying heat transfer unit. The heater and cooler heat transfer units were converted into heat exchangers (HE) by utilizing the output of the process that can be used for other processes so that energy consumption is reduced. The temperature of reaction and the heat transfer unit are modified to reduce energy consumption from 11.850 MMBtu/h to 7.6291 MMBtu/h by changing one heater and one cooler with two heat exchangers.

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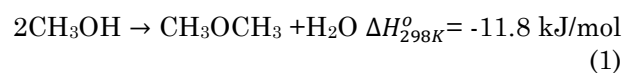
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1. Introduction

Dimethyl ether (DME) production has drawn increasing attention as a promising and clean and environmentally sustainable alternative to diesel fuel [1]. The DME is produced from the variety of feed-stocks such as natural gas, crude oil, residual oil, coal, waste products and bio-mas. Importance of the DME has motivated numerous researches to focus on investigation of various catalysts for methanol dehydration reaction [2].

The dimethyl ether is the simplest ether having the chemical formula of CH₃OCH₃ [3]. DME is used primarily as an aerosol propellant. It

is miscible with most organic solvents, has a high solubility in water, and is completely miscible in water and 6% ethanol. Recently, the use of DME as a fuel additive for diesel engines has been investigated due to its high volatility (desirable for cold starting) and high cetane number. The production of DME is via the catalytic dehydration of methanol over an acid zeolite catalyst. The main reaction of DME production is [4] :



The DME is neither a toxic nor carcinogenic molecule, which is currently used as an aerosol propellant and alternative LPG fuel. The

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suitability of DME as an alternative fuel for diesel engines is well-recognized, thanks to its cleaner emissions with respect to conventional diesel fuel, in terms of SO_x, NO_x, and particulate matter. Furthermore, DME is also considered as a substitute to methanol (MeOH) for both olefins and synthetic-gasoline production. DME is produced from syngas following either an indirect route or direct route [5].

White [6] analyzed and designed the production of DME, the AVEVA Process Simulation software was utilized to simulate the process. The simulation requires 3 heaters and 2 coolers in the equipment configuration so it requires high energy in the process. Heaters are needed for the feed reactor preheater, methanol vaporizer, and the reboiler system in the distillation. Coolers are needed for reactor effluent cooler and column condenser. From these equipment's, a more efficient equipment configuration can be designed by utilizing the output of the process that can be used for other processes so that energy is more efficient. Based on the results of the simulated process run, methanol conversion was obtained at 80%. The methanol conversion was obtained from the process with an operating temperature of 250 °C. However, as the methanol dehydration is a reaction with slightly exothermic, an increase in reaction temperature would decrease in the conversion of methanol. Measured conversion of methanol decreased with an increase in reaction temperature [7].

Many modification have been made in simulation process for the DME synthesis, reactor model, and reaction operational condition in order to increase in the DME production has already been performed [8-9]. In this study, the technological process for the DME synthesis is simulated in Aspen HYSYS based on the combined operating parameters of the reaction dynamic model for methanol dehydration reaction. This paper attempts to evaluate modification on dehydration of methanol process to modify heat transfer unit in order to reduce net energy consumption.

2. Methods

2.1. Process Simulators used for Evaluation

The most popular commercial process simulators are Aspen Plus, Aspen HYSYS, Unisim, VMGSim, ProMax, ChemCad, and so forth. They are very packages capable of solving complex tasks related to process engineering and give chemical engineers the opportunity to make fast and complex calculations [10]. Methods for reducing energy consumption, 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, the Aspen HYSYS simulator provides a thorough thermodynamics basis that allows for precise computation of physical characteristics, transport parameters, and phase behaviour [11]. It is an interactive, intuitive, open and extensible program. It also has many add-on options to extend its capabilities into specific industries. With this program, rigorous steady state and dynamic models for plant design can be created. Apart from that, monitoring, troubleshooting, operational improvement, business planning and asset management can be performed with the aid of the process simulator. Through its completely interactive interface, process variables and unit operation topology can be easily manipulated [12]. Aspen HYSYS offers a comprehensive thermodynamics foundation for accurate calculation of physical properties, transport properties, and phase behavior for the oil & gas and refining industries. Comprehensive library of 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 [13].

2.2 Basic Process Flow Diagram from Literatures

Figure 1 shows the process flow diagram for the dimethyl ether (DME) synthesis [6]. The dimethyl ether is produced by the catalytic dehydration of methanol. Pure methanol (stream 1) is mixed with recycled reactant stream (stream 10), evaporated in the methanol vaporizer E-100, and heated in the reactor feed preheated E-101 before being fed to the reactor CRV-100. The reactor is set to operate at a temperature of 250 °C and 10.75 bar. The effluent from the reactor (stream 6) is cooled by the cooler E-102 before entering the distillation column T-100 at 100 °C and 10 bar. In this column the DME is the distillate and final product, and methanol and water are the bottom product. DME is then cooled in the cooler E-103, and the methanol mixture enters the component splitter X-100, where the water is separated from methanol as the top product and is sent to wastewater treatment to remove traces of organics. Unreacted methanol in the bottom product is recycled and combined with pure methanol in the mixer MIX-100.

The creation of the base case model was executed to accomodate the required annual feed rate of methanol (23,000 tonnes/y). For this process to be successful, the single pass conversion of methanol in the reactor must reach 81% or higher, with a recycle stream being utilized for the unreacted methanol. This

methanol will be returned to the methanol feed and sent back through the process. The product purity of DME must be 99.5% by weight.

2.3. Strategy Modification Heat Transfer Unit

Modifications are made by changing the heater or cooler into a heat exchanger aimed to improve energy efficiency. Heat exchanger, has two functions of heating and cooling [14], can be used to reduce utility consumption in chemical processes which can lead to reduced utility costs and energy consumption [15]. 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 a trade-off between equipment and operating costs may represent the best design for energy efficiency in chemical process plants [16].

Febriana *et al.* [17], conducted research with the pinch method to reduce one stream of cooling water and add two heat exchanger units so that the external energy of both heating and cooling is optimum. Research related to the combination of multi-generation cooling, heating, hydrogen, and poer systems was also conducted by Fang *et al.* [18]. The combination can significantly increase system efficiency so that the energy used is more efficient. The following is a comparison of solar heaters and water heat exchangers with traditional heaters is the initial installation cost of heat exchangers which is higher but has low operating costs compared to ordinary heaters. Heat exchangers can also save energy and long-term cost efficiency [19].

3. Result and Discussion

3.1. Basic Process Flow Diagram and Modification to Reduce Net Energy Consumption

The design capacity of the industrial DME production device from a factory is 15,000 metric

tons of DME per year. The Peng-Robinson-Stryjek-Vera equation of state (PRSV) is used to determine the thermodynamic properties in this study. The PRSV equation has given reliable results for gas phases and polar compounds at a high-pressure system greater than 1 MPa in earlier studies [20]. This fluid package is used for the synthesis gas production unit. The PRSV model is a twofold modification of the Peng-Robinson equation of state that extends the application of the original Peng-Robinson method for moderately non-ideal systems. It is successfully expanded to handle non-ideal systems giving results as good as those obtained using excess Gibbs energy functions like the Wilson, NRTL, or UNIQUAC equations [21].

The dehydration reaction (Equation (1)) was carried out in a fixed bed reactor. Methanol was introduced to the system at 25 °C, 75.43 kgmol/h, and 1.01 bar from methanol synthesis plant. The raw material was mixed with the recycle stream R coming from the separation. Then the pressure was increased to 10.95 bar. This mixture was preheated in the heat exchanger (HE) and vaporized in the heater before entering the reactor. After dehydration, the components in the stream consisted of DME, CH₃OH, and H₂O. The reactor exit stream was used in the heat exchanger (HE) and cooled in the cooler, partially decompressed, and introduced in the distillation tower. DME was obtained in column T-100 with the purity higher than 99.5% (molar basis). The bottoms of column T-100 are fed in the component splitter and that separates water from methanol. Water was sent to a heat exchanger (HE) to reduce the temperature of DME then sent to a treatment section, while the methanol was recycled.

Modifications were made by changing the heater or cooler into a heat exchanger aimed to improve energy efficiency as depicted in Figures 3-6, while mass and energy balances is reported in Table S1 (Supporting Information (SI)). The chemical reaction in the reactor CRV-100 is exothermic, which in turn the heat is generated

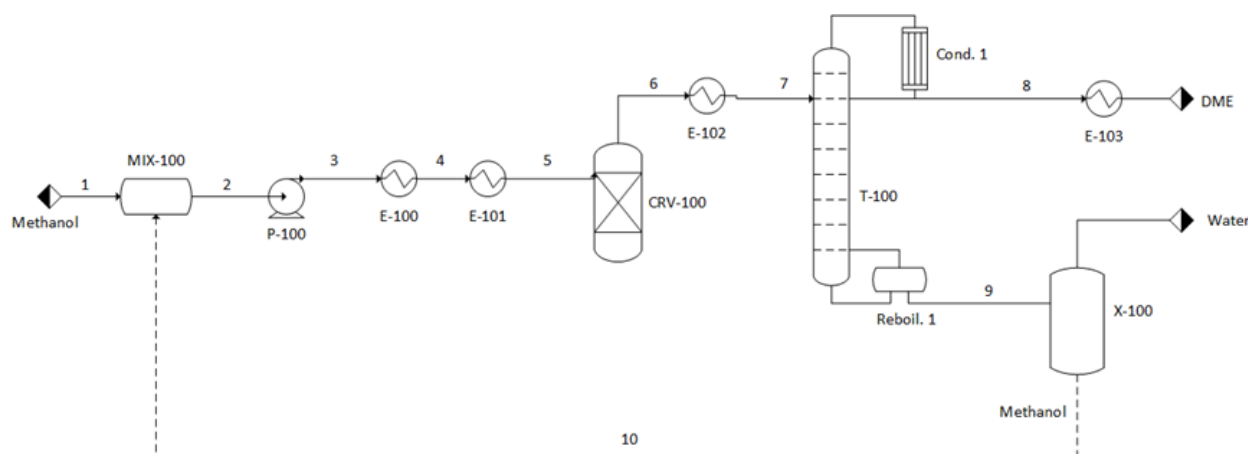


Figure 1. Process Flow Diagram (PFD) for the conversion of methanol to dimethyl ether (DME)

and released that used to heating source. Then the heat exchanger E-103 in Figure 5 replaced the cooler E-103 in Figure 3 which uses cooling water to reduce the temperature before the flow becomes product.

3.2. Thermodynamics and Operating Conditions Consideration

Based on Ardy *et al.* [7] and Liu *et al.* [22], as the methanol dehydration is a reaction with slightly exothermic, an increase in reaction temperature would decrease in the conversion of

methanol. Measured conversion of methanol decreased with an increase in reaction temperature. DME is typically obtained via methanol dehydration (Equation (1)) in gas phase over acid catalysts, such as $\gamma\text{-Al}_2\text{O}_3$, zeolites or silica-modified alumina, at moderate pressures (10-20 bar) [23]. Methanol dehydration was the main reaction and the methanol decomposition occur in the temperature range between 200–400 °C. Methanol reacts more selectively to form DME at temperature closes to 200 °C [24].

The DME synthesis reaction (Equation (1)) from modified methanol dehydrogenation occurs

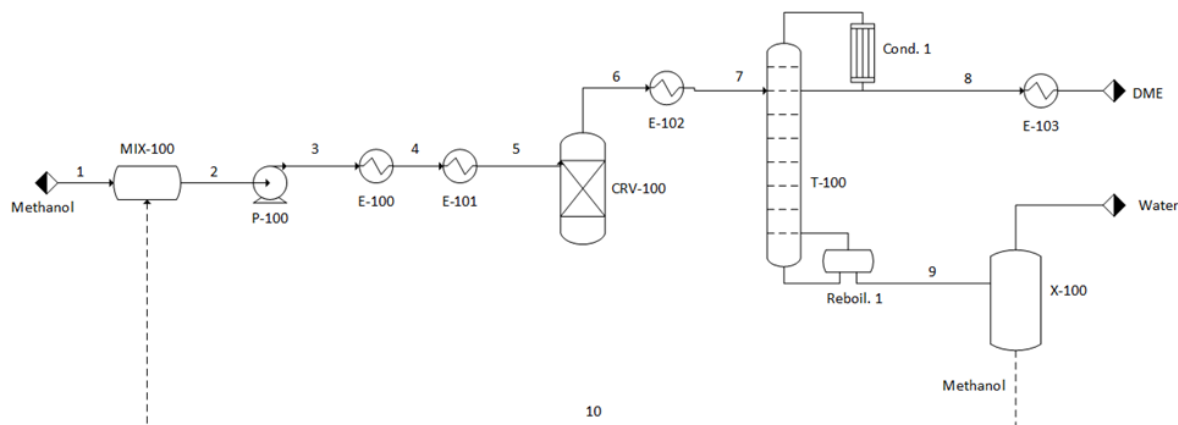


Figure 3. Process Flow Diagram (PFD) of basic process before process modifications

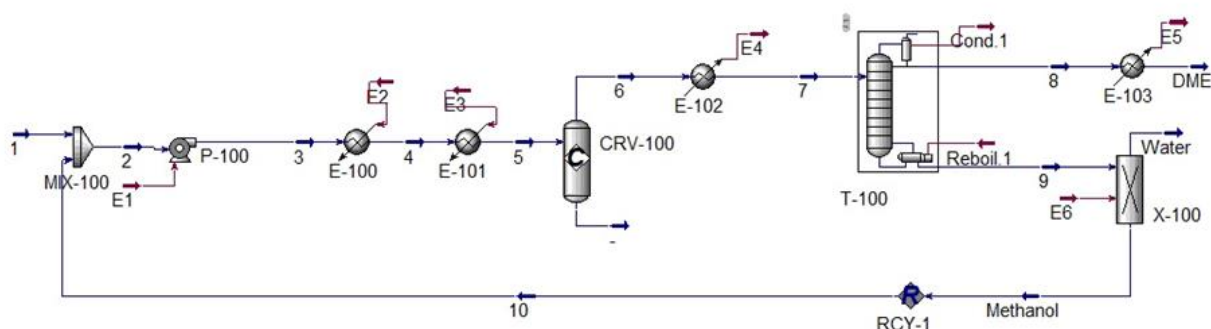


Figure 4. Aspen HYSYS simulation of basic process before modifications

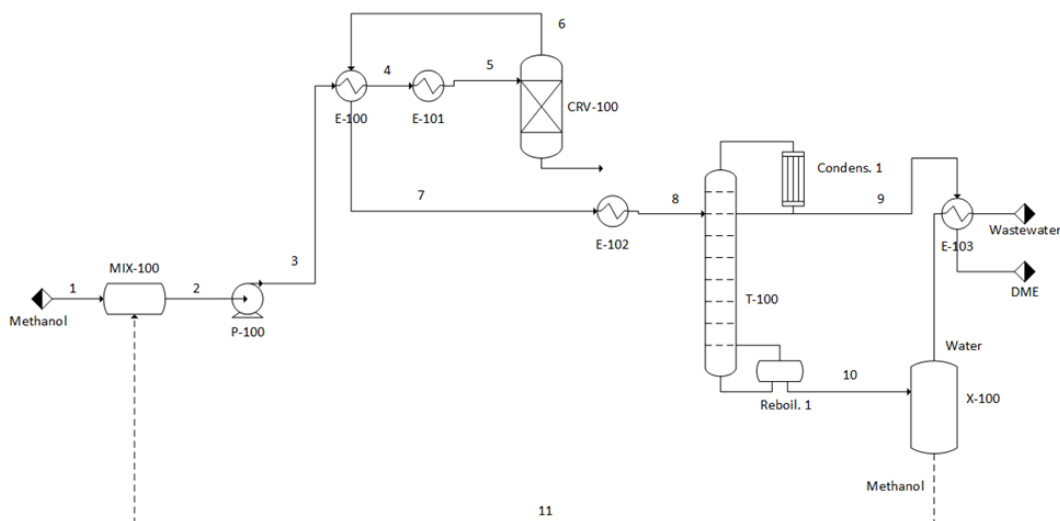


Figure 5. Process Flow Diagram (PFD) of modified process

at 200 °C and 10.75 bar. 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.

Heat of reaction ΔH_{298K}^o

The data of ΔH_{298K}^o for each component in the dehydrogenation reaction of methanol to dimethyl ether is as follows [25]:

$$\Delta H_{298K}^o \text{ CH}_3\text{OH} = -201.17 \text{ kJ/mol}$$

$$\Delta H_{298K}^o \text{ CH}_3\text{OCH}_3 = -184.1 \text{ kJ/mol}$$

$$\Delta H_{298K}^o \text{ H}_2\text{O} = -241.8 \text{ kJ/mol}$$

$$\begin{aligned} \Delta H_{298K}^o &= \Delta H_{f, 298 K, \text{ product}} - \Delta H_{f, 298 K, \text{ reactant}} \\ &= [-184.1 \text{ kJ/mol} + (-241.8 \text{ kJ/mol})] - [2 \times (-201.17 \text{ kJ/mol})] = -23.56 \text{ kJ/mol} \end{aligned}$$

Based on these calculations, the ΔH value shows a negative price (-) so that the reaction is an exothermic reaction or a reaction that produces heat. If the operating temperature is higher, the conversion decreases. Therefore, to keep the reaction going according to the operating conditions, cooling is necessary.

Gibbs Free Energy

The data of ΔG_{298K}^o for each component in the dehydrogenation reaction of methanol to dimethyl ether is as follows [25]

$$\Delta G_{298K}^o \text{ CH}_3\text{OH} = -162.51 \text{ kJ/mol}$$

$$\Delta G_{298K}^o \text{ CH}_3\text{OCH}_3 = -112.9 \text{ kJ/mol}$$

$$\Delta G_{298K}^o \text{ H}_2\text{O} = -228.6 \text{ kJ/mol}$$

$$\begin{aligned} \Delta G_{298K}^o &= \Delta G_{f, 298 K, \text{ product}} - \Delta G_{f, 298 K, \text{ reactant}} \\ &= [-112.9 \text{ kJ/mol} + (-228.6 \text{ kJ/mol})] - [2 \times (-162.51 \text{ kJ/mol})] \end{aligned}$$

Therefore, $\Delta G_{298K}^o = -16.48 \text{ kJ/mol}$

From the above calculation, a result of $\Delta G_{298K}^o = -16.48 \text{ kJ/mol}$ is obtained, so this reaction takes place spontaneously because the result obtained from the calculation of $\Delta G_{298K}^o < 0$.

$$\ln K_{298} = \frac{-\Delta G}{R T} = \frac{-(-16480 \text{ J/mol})}{8.314 \frac{\text{J}}{\text{mol.K}} \times 298 \text{ K}} = 6.652$$

$$K_{298} = 774.331$$

$$\ln \frac{K_{473}}{K_{298}} = -\frac{\Delta H_{298K}^o}{R} \times \left(\frac{1}{T_{473}} - \frac{1}{T_{298}} \right)$$

$$\ln \frac{K_{473}}{774.331} = -\frac{-23560 \text{ J/mol}}{8.314 \frac{\text{J}}{\text{mol.K}}} \times \left(\frac{1}{473 \text{ K}} - \frac{1}{298 \text{ K}} \right)$$

$$\ln \frac{K_{473}}{774.331} = -3.518$$

$$\text{Thus, } K_{473} = 22.966$$

The equilibrium value of the reaction at an operating temperature of 200 °C is obtained equal to 22.966 so that the reaction is an irreversible reaction.

3.3. Reduced Energy Consumption by Process Modification

In this study, the heat transfer unit of the methanol dehydration process was modified. The heat transfer unit was modified by changing one heater and cooler to two heat exchangers (HE). Heat transfer unit modification with fixed pressure can result in reducing energy consumption so that reduce production cost. The

Table 1. Modification effect in heat transfer unit

Energy stream	Energy before modification (MMBtu/h)	Energy after modification (MMBtu/h)
E1	0.0048	0.0048
E2	4.4380	-
E3	0.6210	3.3850
E4	3.4868	1.8160
E5	0.0626	-0.7367
E6	-0.6205	-
Cond.1	1.8974	1.8940
Reboil.1	1.2679	1.2660
Total	11.850	7.6291

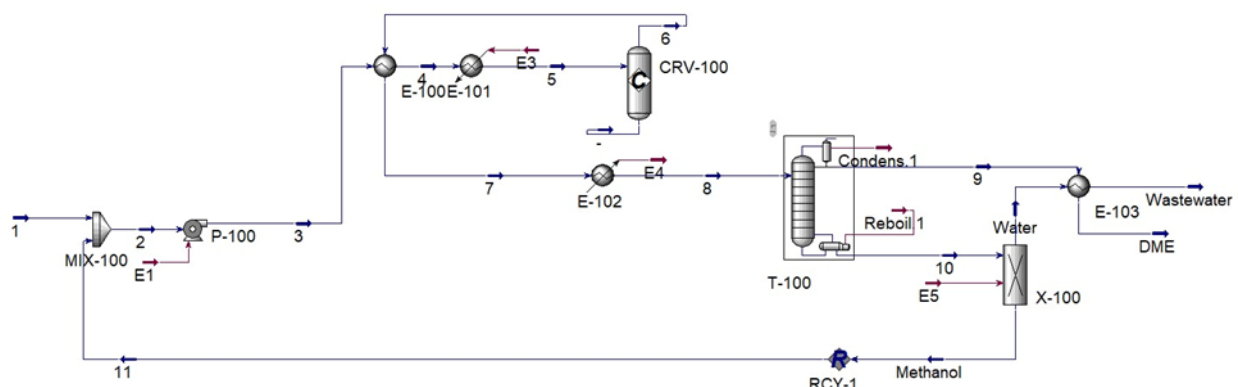


Figure 6. Aspen HYSYS simulation of the modified process

energy consumption is reduced from 11.850 MMBtu/h to 7.6291 MMBtu/h (Table 1).

4. Conclusion

Simulation of a DME plant which is capable of producing DME with high purity (15,000 tons per year) from methanol was done using Aspen HYSYS process simulator. The PRSV is chosen as the property method in the simulation. Energy consumption of simulation is reduced from 11.850 MMBtu/h to 7.6291 MMBtu/h by changing one heater and one cooler with two heat exchangers. Based on the findings, it was concluded that production of DME from methanol dehydration with lower net energy consumption is technically feasible. Further research into parameter changes and energy integration is necessary to optimize the process profitability.

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