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Research Article

Enhancing Energy Efficiency in Methanol-to-DME Conversion through Process Modification and Heat Integration

Salma Salsabila[1]*, Meirisa Ayu Saputri[1], Jorsch Pieter Benhard Sirait[1], Samuel Kurniawan[1], Sera Amelia[1], Alvin Ananta Putra[2]

[1]Department of Chemical Engineering, Faculty of Engineering, Universitas Diponegoro, Semarang 50275, Indonesia.
[2]Department of Chemical Engineering, Faculty of Engineering, Universitas Gadjah Mada, Yogyakarta, Indonesia.

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Abstract

Enhancing energy efficiency in dimethyl ether (DME) production is critical for reducing utility consumption and improving process sustainability. This study investigates the impact of targeted modifications to the methanol dehydration system on thermal performance and operational stability. The proposed configuration incorporates an expanded heat-integration network, additional feed-conditioning units, and a split-recycle arrangement to optimize energy recovery and maintain reactor stability. A water knock-out vessel and supplementary exchangers were also integrated to improve separation efficiency and reduce reboiler duty. Comparative process simulations were performed using with the NRTL thermodynamic model to evaluate the baseline and modified flowsheets. Results indicate that the optimized design achieves a 35.55% increase in energy efficiency while preserving the original methanol conversion level of 50.35%, confirming that reduced energy demand does not compromise reaction performance. These findings demonstrate that the proposed modifications provide a more energy-efficient and industrially viable configuration for DME production, offering a strong foundation for future optimization and process intensification strategies.

Keywords: Energy Efficiency; Dimethyl Ether; Heat Integration; DME

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1. Introduction

Dimethyl Ether (DME), with the chemical formula CH_3OCH_3, has emerged as a compound of considerable significance within both the chemical and energy industries [1]. Historically, DME has been utilized as a critical feedstock in the synthesis of olefins, methyl tert-butyl ether (MTBE), and other high-value chemical intermediates [2]. In recent years, its application has extended to the energy domain, where it is recognized for its potential as a clean-burning alternative fuel, a feedstock for fuel cells, and a hydrogen carrier within methanol-based energy systems [3]. The key reaction in the synthesis of dimethyl ether (DME) is the catalytic dehydration of methanol. This transformation can be described by the following chemical equation:

$$2CH_3OH \rightleftarrows CH_3OCH_3 + H_2O \qquad \Delta H^\circ_{298} = -23.56\ \text{kJ/mol} \qquad (1)$$

Industrial synthesis of dimethyl ether (DME) is primarily conducted via the catalytic dehydration of methanol, a process that inherently involves water formation or interaction depending on the specific configuration employed [4]. Although the methanol-to-DME pathway is well established, it remains constrained by significant operational challenges, most notably its high energy intensity [5]. Substantial thermal input is required to preheat and vaporize the methanol feed, maintain the endothermic reaction environment, and achieve efficient separation of

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* Corresponding Author.
Email: salma.undip1@gmail.com (S. Salsabila)

methanol–water–DME mixtures in downstream purification units. These requirements collectively impose considerable utility demands and elevate operating costs, thereby positioning energy optimization as a critical priority in DME process design [6]. Recent investigations have highlighted pronounced thermal losses and elevated reboiler duties within separation systems, underscoring the necessity of advanced heat-integration strategies to mitigate overall energy consumption [7]. Furthermore, process analyses indicate that the configuration of separation and recycle units can exacerbate energy intensity, as schemes incorporating light-gas recycling typically require increased heating and cooling duties, reinforcing the imperative for process-level optimization to minimize utility loads [8].

In light of these considerations, the present study is directed toward optimizing dimethyl ether (DME) production from methanol and water by reducing the overall energy intensity of the process. This objective is pursued through the application of rigorous process simulation and systematic modifications to key operational units, particularly those associated with heating, cooling, and separation. The aim is to develop an energy-efficient flowsheet that preserves product purity and reaction performance while ensuring operational reliability and economic feasibility.

2. Method

2.1. Process Simulators Used for Evaluation

Process simulation tools constitute a fundamental component in the evaluation of the methanol dehydration pathway for dimethyl ether (DME) production, as they provide a controlled and highly adaptable framework for analyzing complex thermodynamic and kinetic interactions within the system. Advanced platforms such as Aspen HYSYS integrate sophisticated optimization algorithms, encompassing both linear and nonlinear programming, alongside sensitivity analysis capabilities, thereby enabling the simultaneous consideration of economic, environmental, and operational objectives in process design [9]. These simulators employ rigorous thermodynamic models, including Peng–Robinson and Non-Random Two-Liquid (NRTL), which are essential for accurately predicting vapor–liquid equilibria in multicomponent systems comprising methanol, water, and DME. Through detailed modeling, sensitivity analyses can be performed on critical variables such as temperature, pressure, catalyst performance, and feed composition, facilitating the identification of optimal operating conditions. This simulation-based approach significantly reduces reliance on early-stage experimental trials, conserving time, raw materials, and operational costs while ensuring high predictive accuracy.

In addition to steady-state analysis, process simulators provide dynamic modeling capabilities that are critical for assessing process controllability, start-up and shut-down behavior, and overall operational stability in methanol-to-DME production systems. Advanced functionalities, such as pressure-swing simulations, energy-optimization modules, and automated design-specification tools, enable the identification of process bottlenecks and support improvements in conversion efficiency within the DME dehydration reactor. Furthermore, integrated economic analysis frameworks facilitate concurrent evaluation of utility consumption, equipment sizing, and total cost estimation, thereby ensuring that proposed designs are both technically robust and economically viable. By combining rigorous thermodynamic assessment, comprehensive process modeling, and systematic techno-economic evaluation, studies such as that of Domingos et al. reaffirm the indispensable role of process simulators in the development of optimized and resilient methanol–DME production processes [7].

2.2. Description of Process

Methanol (CH_3OH), commonly referred to as methyl alcohol, is a fundamental platform chemical extensively employed in the synthesis of olefins, dimethyl ether (DME), methyl tert-butyl ether (MTBE), and a wide range of other industrial chemicals [10]. Approximately 85% of global methanol production is consumed in the manufacture of chemical intermediates; however, recent studies have also emphasized its potential as an alternative fuel for internal combustion engines due to its favorable combustion characteristics. From a chemical standpoint, methanol is primarily produced from synthesis gas, a mixture of CO, CO_2, and H_2, via catalytic hydrogenation reactions [11]. In response to global decarbonization initiatives, alternative and renewable production routes, including biomass conversion, CO_2 hydrogenation, and DME-based processes, have attracted increasing attention. Beyond its conventional industrial applications, methanol is gaining strategic importance in the energy sector as a clean-burning fuel, a feedstock for fuel cells, and a hydrogen carrier within methanol economy frameworks. Despite these advantages, methanol presents significant health hazards, as it is toxic when ingested, inhaled, or absorbed through the skin, necessitating strict handling and safety protocols. Nevertheless, its combination of high chemical reactivity, relatively low production cost, and broad application portfolio ensures that methanol remains a cornerstone of both traditional and emerging sustainable chemical industries. The chemical reaction is following Equation (1).

2.3. Method to Improve Net Energy Efficiency of Dimethyl Ether (DME) Production

Energy represents a fundamental requirement in industrial operations, as virtually all processes are highly dependent on its availability. Ensuring reliable access to energy, whether in the form of electricity or conventional fuels such as coal, charcoal, and firewood is essential for maintaining continuous production. One of the most effective strategies for reducing energy consumption is process optimization, which can be achieved through improvements in equipment efficiency and systematic design modifications. In the context of dimethyl ether (DME) production, these modifications primarily aim to minimize net energy demand by incorporating heat recovery systems. Specifically, the integration of heat exchangers can reduce the thermal load on cooling units, while repurposing hot wastewater for preheating feed streams prior to entering the heater further enhances energy utilization. Collectively, these measures contribute to lowering utility requirements and operational costs, thereby improving the sustainability and economic viability of the process.

In this study, energy savings are quantified as the percentage reduction in total external utility demand resulting from process modifications (Equation (2)). $E_{\text{unmodified}}$ denotes the total utility consumption of the base-case process configuration, which operates without process-level heat integration and relies exclusively on conventional heating and cooling utilities. This demand encompasses the energy required for feed pressurization, methanol vaporization and preheating prior to reactor entry, reactor temperature control, cooling and partial depressurization of the reactor effluent, as well as the reboiler and condenser duties associated with distillation-based separation units. By contrast, E_{modified} represents the total external utility consumption following the implementation of heat-integration and process-intensification measures, including staged feed preheating, recovery of thermal energy from the reactor effluent, recycle-stream conditioning, integration of a water knock-out unit, and enhancements within the separation train. Accordingly, E_{modified} reflects the net heating and cooling utility requirements after accounting for internal energy recovery within the process.

$$Energy\ Saving\ (\%) = \frac{E_{unmodified} - E_{modified}}{E_{unmodified}} \times 100\% \qquad (2)$$

3. Results and Discussion

3.1. Basic Unmodified PFD Analysis

The industrial dimethyl ether (DME) production facility considered in this study has a design capacity of 50,000 metric tons per year as a case study (Figure 1). To accurately represent phase behavior and thermodynamic interactions, the Non-Random Two-Liquid (NRTL) model is employed. The dehydration reaction is conducted within a multistage reactor configuration. The methanol feed enters the system at 25 °C, with a flow rate of 262 kmol.h^{-1} and an initial pressure of 100 kPa. Subsequently, the system pressure is increased to 1,400 kPa. The fresh feed is combined with a recycle stream (R) originating from the separation section, after which the blended stream undergoes vaporization in the heater and is further preheated via a heat exchanger prior to introduction into the reactor.

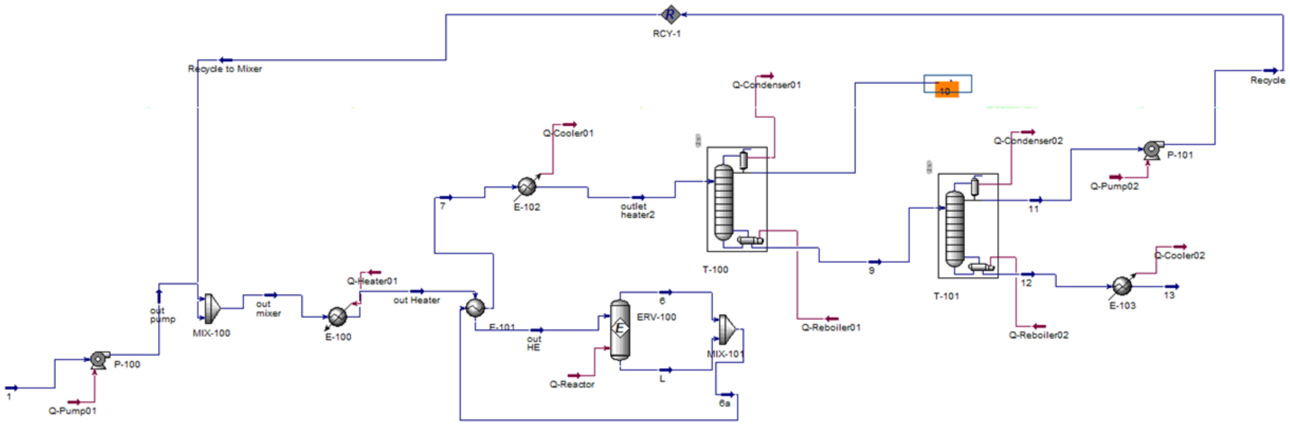

Figure 1. Unmodified flow diagram to be simulated using HYSYS simulator [12].

The post-dehydration stream comprises dimethyl ether (DME), unreacted methanol (CH_3OH), water (H_2O), and trace impurities. The reactor effluent is subsequently cooled, partially depressurized, and directed to the separation section. The primary distillation column (T-100) produces DME with a purity exceeding 99.9%, while the column bottoms are expanded and routed to a secondary distillation column for methanol–water separation. The recovered water is transferred to a purification unit to remove residual organic contaminants, whereas the methanol stream is recycled to the reactor feed. The condenser of the DME column operates using cooling water, and the implementation of additional cryogenic refrigeration is not recommended due to economic and operational considerations.

3.2. Enhancing Energy Efficiency Through Process Modifications

In this study, targeted modifications were implemented in the heat-transfer network integrated into the methanol dehydration process for dimethyl ether (DME) production (Figure 2). The revised flowsheet introduces structural and operational improvements aimed at enhancing overall process efficiency relative to the baseline configuration. Specifically, the design incorporates an expanded heat-integration scheme comprising additional preheaters and heat exchangers (E-104, E-105, E-101, and E-103), which facilitate effective recovery of thermal energy from the reactor effluent and controlled preheating of the reactor feed. This staged heating strategy significantly reduces external utility requirements and ensures stable inlet conditions for the methanol dehydration reactor, which is highly sensitive to temperature variations [1].

A water knock-out vessel (V-100) is incorporated upstream in the recycle loop to enable early removal of condensed water, thereby improving downstream separation efficiency and reducing moisture-related operational issues. Furthermore, the modified flowsheet adopts a split-recycle configuration (RCY-1 and RCY-2), which provides enhanced flexibility in controlling recycle composition and temperature, ultimately promoting higher conversion in this equilibrium-limited reaction [2]. Additional mixers and conditioning units (MIX-101 and MIX-102) are employed to ensure thermal and compositional uniformity prior to reactor entry, while supplementary heat exchangers integrated within the separation train reduce reboiler duty and deliver drier purge and recycle streams. Collectively, these modifications exemplify established chemical engineering strategies for energy intensification and process optimization, resulting in a more controllable, energy-efficient, and industrially representative DME production system. Collectively, these modifications reflect established chemical-engineering strategies for intensifying energy use, resulting in a more controllable, energy-efficient, and industrially representative DME production process (Figure 2).

3.3. Thermodynamic Framework and Operating Condition Analysis

The operating conditions are defined by considering both thermodynamic viability and the expected performance of the reactor and separation units. In this design, the dehydration reactor is operated at approximately 1400 kPa to

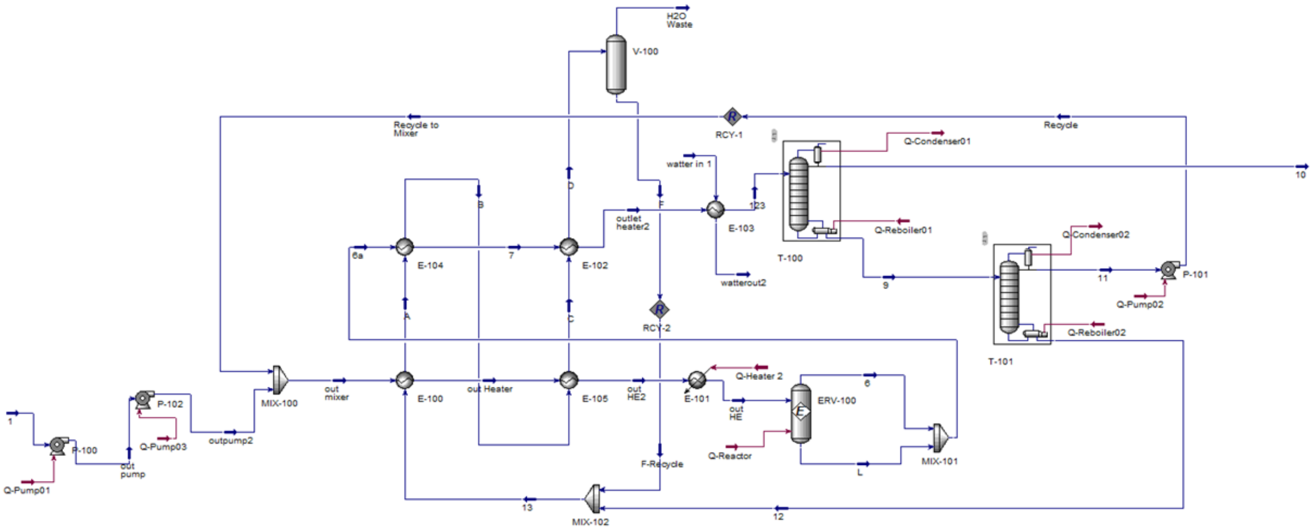

Figure 2. Modified flow diagram to be simulated using HYSYS simulator.

ensure that the feed and products remain fully in the vapor phase. Maintaining vapor-phase conditions is critical for solid acid catalysts such as γ-Al_2O_3 and ZSM-5, as operating prior to any condensation ensures efficient deoxygenation, minimizes the deposition of heavy oxygenates on the catalyst surface, and slows deactivation, thereby preserving overall catalytic performance [13]. Because DME synthesis is equilibrium-limited, maintaining a stable inlet temperature is essential. Even small temperature deviations can shift the equilibrium position and noticeably influence methanol conversion and overall DME yield [14].

On the separation side, the vapor–liquid equilibrium behavior of the DME–MeOH–H_2O mixture supports the use of moderate distillation pressures. Based on its highest volatility, DME can be selectively removed as the overhead product, while the heavier components remain in the lower sections of the column, consistent with the phase-equilibrium characteristics [15]. In contrast, the methanol–water mixture, which shows strong non-ideal interactions, requires a dedicated bottom-section purification step accompanied by a recycle loop to reach the specified product quality. Such a configuration is consistent with findings reported in studies of methanol dehydration and VLE behavior in DME production [16]. Overall, these thermodynamic considerations, which include phase behavior, reaction equilibrium, and differences in volatility, determine the practical operating window of the integrated process and contribute to stable and reliable performance of the DME production plant.

3.4. Thermodynamics Review

A comprehensive assessment of the system's thermodynamic characteristics is essential for determining how heat flow and energy distribution influence overall process performance, particularly through the evaluation of enthalpy changes ($\Delta H°_{298K}$) and Gibbs free energy ($\Delta G°_{298K}$) [17]. By evaluating the interplay among temperature, pressure, enthalpy variation, and equilibrium conditions, the analysis identifies the primary factors that influence reaction viability and energy efficiency. Furthermore, evaluating equilibrium behavior through ΔG° provides insight into the reaction's feasibility and degree of reversibility, offering a clearer understanding of how variations in operating conditions can shift the equilibrium and influence overall process stability [18]. The resulting understanding serves as a foundation for optimizing the system to minimize energy losses and enhance operational reliability [19]. The value of $\Delta H°_f$ and $\Delta G°_f$ [20] can be seen in Table 1.

The dehydration of methanol can be expressed as [5]:

$$2CH_3OH \rightleftharpoons CH_3OCH_3 + H_2O$$

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

$$\Delta H°_{298K} = \sum \Delta H_f^{\circ} \text{product} - \sum \Delta H_f^{\circ} \text{reactant}$$

$$\Delta H°_{298K} = (\Delta H_f^{\circ}\, CH_3OCH_3 + \Delta H_f^{\circ}\, H_2O) - 2(\Delta H_f^{\circ}\, CH_3OH)$$

$$\Delta H°_{298K} = -23.56 \text{ kJ/mol}$$

Based on the calculation, the result is determined to be negative, indicating that the reaction is exothermic, indicating that heat is released during the process. Higher operating temperatures can shift the equilibrium unfavorably and diminish conversion efficiency. Accordingly, temperature regulation through adequate cooling is essential to sustain optimal reaction conditions [21].

$$\Delta G°_{298K} = \sum \Delta G_f^{\circ} \text{product} - \sum \Delta G_f^{\circ} \text{reactant}$$

$$\Delta G°_{298K} = (\Delta G_f^{\circ}\, CH_3OCH_3 + \Delta G_f^{\circ}\, H_2O) - 2(\Delta G_f^{\circ}\, CH_3OH)$$

$$\Delta G°_{298K} = -16.51 \text{ kJ/mol}$$

The negative standard Gibbs free energy change at 298 K verifies that the methanol dehydration reaction proceeds spontaneously under standard conditions [15].

$$\ln K_{298} = \frac{-\Delta G}{RT} = 6.664 \text{ and } K_{298} = 783.679$$

At the reaction temperature of 634.6 K, the equilibrium constant (K) is $K_{634.6} = 1.215 \times 10^5$. At the reaction temperature of 634.6 K (361.4 °C), the Gibbs free energy change is given by:

$$\Delta G_{634.6\,K} = -R \times T_{634.6\,K} \times \ln K_{634.6\,K} = -61.77 \text{ kJ/mol}$$

The negative Gibbs free energy change at the reaction temperature indicates that the methanol dehydration reaction is thermodynamically favorable under the investigated operating conditions. At the operating temperature of 634.6 K (361.4 °C), the reaction equilibrium constant reaches a value of 1.215×10^5. A high equilibrium constant (K) indicates that, at equilibrium, the

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

Compound	ΔH_f° (kJ/mol)	ΔG_f° (kJ/mol)
Methanol	-201.17	-162.51
Dimethyl Ether	-184.1	-112.93
Water	-241.8	-228.6

ratio of product concentrations to reactant concentration is strongly shifted toward the products. This demonstrates that the thermodynamic equilibrium inherently favors DME formation, thereby implying that the maximum attainable conversion is more strongly governed by kinetic constraints or reactor design considerations than by equilibrium limitations [22].

3.5. Energy Analysis between Unmodified and Modified Process

An energy analysis was conducted to quantify the improvement in thermal performance achieved by the modified process relative to the original configuration. The evaluation encompassed heating and cooling loads, the degree of heat-integration implemented, and the corresponding reduction in overall utility consumption. The total energy saving was calculated by directly comparing the summed heating and cooling duties reported by Aspen HYSYS for both process configurations, without additional manual correction factors. The results indicate that the modified configuration achieves a 35.55% increase in energy efficiency while maintaining the original process conversion level at 50.35%. This finding demonstrates that the reduction in energy demand does not compromise reaction performance, thereby validating the effectiveness of the optimization strategy. For clarity, the calculated energy metrics for both process configurations are presented in Table 2. The tabular representation enables a direct comparison of total energy requirements and the distribution of utility loads across individual process units. These data serve as the basis for evaluating the overall impact of the implemented modifications on thermal performance and energy efficiency.

4. Conclusion

Process modification in DME production shows a substantial improvement in overall energy use. The modifications implemented in the flowsheet enhance heat recovery, reduce external utility demand, and create a more thermally efficient operation compared with the unmodified process. Based on the overall energy analysis, the modified process demonstrates an energy-efficiency improvement of approximately 35.55%, indicating a significant reduction in total heating and cooling requirements. Further evaluation of the system is still needed to explore additional optimization opportunities and to ensure stable performance under different operating conditions, especially as energy efficiency continues to be a key priority in modern chemical-process design.

CRedit Author Statement

Author Contributions: S. Salsabila: Writing draft preparation, review, editing, data curation, validation, writing and final manuscript revision, and supervision; J.P.B. Sirait: Conceptualization, methodology, formal analysis, visualization; M.A. Saputri: Methodology, conceptualization, software, investigation, resources; S. Kurniawan: Conceptualization, methodology, formal analysis, data Curation, Visualization; S. Amelia: Investigation, resources, writing, review and editing, software; A.A. Putra: : Investigation, resources, writing, conceptualization. All authors have read and agreed to the published version of the manuscript.

Table 2. Energy analysis of the unmodified and modified process.

Unmodified Process		Modified Process	
Heat stream items	Heat flow (kJ/h)	Heat stream items	Heat flow (kJ/h)
Q-Cooler01	4.059E8	Q-Cooler01	-
Q-Cooler02	4.252E7	Q-Cooler02	-
Q-Condenser01	1.273E8	Q-Condenser01	1.177E8
Q-Condenser02	2.003E8	Q-Condenser02	1.855E8
Q-Heater01	3.906E8	Q-Heater01	-
Q-Heater 2	-	Q-Heater 2	3.437E8
Q-Reboiler01	1.393E8	Q-Reboiler01	1.239E8
Q-Reboiler02	2.011E8	Q-Reboiler02	1.862E8
Q-Pump01	6.574E5	Q-Pump01	1.360E5
Q-Pump02	9.077E4	Q-Pump02	9.077E4
Q-Pump03	-	Q-Pump03	5.214E5
Q-Reactor	2.290E7	Q-Reactor	2.290E7
Total	1.531E9	Total	9.806E8

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