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Journal of Chemical Engineering Research Progress, 2 (2) 2025, 284-289

Research Article

Design and Simulation of High-Yield Dimethyl Ether Synthesis Using Series Reactors and Intercooler

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Received: 11th December 2025; Revised: 15th December 2025; Accepted: 17th December 2025
Available online: 24th December 2025; Published regularly: December 2025

Abstract

Dimethyl ether (DME, CH_3OCH_3), the simplest alkyl ether and a structural isomer of ethanol, has attracted considerable attention as a clean fuel and chemical intermediate. To enhance its production efficiency, process modifications were introduced and rigorously evaluated through simulation modeling. The methodology involved systematic optimization of operating parameters to achieve targeted performance criteria. A key innovation was the adoption of a series-reactor configuration integrated with an intercooler between reactors, designed to improve conversion and yield. The modified process demonstrated a substantial improvement in DME production, with yield increasing from 40.87% to 62.29%. These results confirm that the proposed process modification significantly augments both yield and conversion, thereby offering a more efficient and sustainable route for DME synthesis.

Keywords: dimethyl ether; process modification; reactor; intercooler

How to Cite: Nurfiana, S. A., Shofa, F. Z., Larasati, L., Dayita, Y., Cahyaningsih, S. (2025). Design and Simulation of High-Yield Dimethyl Ether Synthesis Using Series Reactors and Intercooler. *Journal of Chemical Engineering Research Progress*, 2 (2), 284-289 (doi: 10.9767/jcerp.20568)

Permalink/DOI: https://doi.org/10.9767/jcerp.20568

1. Introduction

Dimethyl ether (DME) is a clean and efficient energy substitute with vast potential for applications across the chemical industry [1]. Dimethyl ether (DME, CH_3OCH_3), the simplest ether, can be produced on an industrial scale from a variety of carbon-based feedstocks, including petroleum, coal, and biomass, as well as from valuable by-products such as methanol and hydrogen. This compound is a colourless, odourless gas, first synthesized in 1835 by chemists Jean-Baptiste Dumas and Eugene Péligot through the distillation of methanol in the presence of sulphuric acid [2]. The modification process to improving net energy of production styrene can be modified in a various way. In this study, heat exchanger is used to substitute the cooler and heater to improve the net energy [3]. In contemporary industrial practice, DME is synthesized from a range of feedstocks, including natural gas, methanol, biomass, and coal. Its exceptionally low boiling point and absence of sulphur are key physicochemical attributes that underscore its growing relevance, particularly as a solvent in both chemical and petrochemical processes [4]. Dimethyl ether (DME) is a clean and efficient energy substitute with vast potential for applications across the chemical industry [1]. Dimethyl ether (DME, CH_3OCH_3), the simplest ether, can be produced on an industrial scale from a variety of carbon-based feedstocks, including petroleum, coal, and biomass, as well as from valuable by-products such as methanol and hydrogen. This compound is a colourless, odourless gas, first synthesized in 1835 by chemists Jean-Baptiste Dumas and Eugene Péligot through the distillation of methanol in the

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Initially, DME was produced unintentionally as a by-product of high-pressure methanol synthesis operating at around 300 bar. With the introduction of low-pressure methanol synthesis technologies in the 1960s, the need for a dedicated process specifically designed for DME production became evident. Today, industrial facilities that exclusively dehydrate methanol to produce DME are already in operation, and the global market capacity has reached approximately 4 million tonnes per year. Demand for DME has generally increased over recent years, with the only decline occurring in 2020 due to the global economic slowdown caused by the COVID-19 pandemic. In the coming years, the DME market is projected to continue expanding, reaching an estimated production level of about 9.5 million tonnes per year by 2027 [2,5].

Dimethyl ether is a simple ether that has attracted attention as a clean fuel and platform chemical due to its favourable physical and chemical characteristics. Under standard conditions, DME is a gas, but it can be stored as a liquid under low pressure, facilitating transport and distribution. DME exhibits combustion properties that reduce particulate and sulphur emissions compared to diesel fuel, making it a potential substitute for LPG, aerosol propellants, and clean diesel fuel in various transportation and household applications [3]. In addition, its high cetane value and auto-ignition characteristics make DME compatible with modified diesel engines and alternative combustion systems, expanding its industrial role in the energy and transportation sectors [6]. In the last 10 years, one of the most promising technologies is the use of methanol as a C1 building block in the petrochemical industry, and a wide part of its production is consumed in the manufacturing of DME as an alternative fuel. DME has an octane number and ignition temperature close to that of diesel fuel. It leads to lower NOX emissions, less smoke, and less engine noise than conventional diesel engines [7].

The indirect synthesis of dimethyl ether (DME) is conventionally carried out in a single adiabatic fixed-bed reactor employing γ-Al_2O_3 as the catalyst. Previous studies have primarily concentrated on catalyst development, operating condition optimization, and process intensification through advanced separation technologies. Although this configuration can achieve high product purity, overall conversion and yield remain constrained by thermodynamic equilibrium limitations and the significant temperature rise associated with the reaction's exothermic nature [5]. To overcome these challenges, the present study proposes a novel reactor-in-series configuration for the dehydration step. By enabling improved temperature regulation and facilitating stepwise equilibrium shifting along the reaction pathway, this design is expected to enhance DME yield without altering the catalyst type or adding complexity to downstream separation units.

2. Methods

2.1. Process Simulators Used for Evaluation

Process simulation is a vital component of process engineering, as it enhances system control and maintenance in the face of operational challenges, regulatory demands, and market competition. Simulator software tools, such as Aspen Plus, Aspen HYSYS, and similar simulators, are indispensable for building precise models that help engineers understand plant behavior under various operating conditions [8]. These tools provide engineers with the capability to handle complex calculations quickly and effectively [9]. Aspen HYSYS is a process-simulation platform extensively employed across the petroleum, natural gas, and refining sectors due to its rigorous thermodynamic framework, which supports precise evaluation of physical properties and phase behavior [10]. The software encompasses a broad selection of thermodynamic models, allowing engineers to determine the most suitable approach for conducting analyses related to phase equilibria and enthalpy of chemical species. In the present simulation of the ethylbenzene dehydrogenation process for styrene manufacture, the Peng–Robinson (PR) equation-of-state package was selected as the thermodynamic basis to facilitate optimization activities.

2.2. Description of Process

There are two main ways to produce DME: the first, which is tje historical one, is the indirect route where DME is obtained by the dehydration of methanol and the second, which is more efficient, is the direct route where DME is produced directly from syngas in a single stage

tank to bifunctional catalysts. For both routes, the feedstock can be coal, natural gas, oil or biomass.

2.2.1. Indirect method

Historically, DME has been produced from syngas in a two-step process: methanol is first produced and purified and then converted to DME in a second reactor. The conversion of methanol to DME occurs through a dehydration as seen in the following equation:

$$2CH_3OH \rightarrow CH_3OCH_3 + H_2O \; \Delta H^o_{298K} = -23.5 \text{ kJ/mol} \quad (1)$$

Theoretically, as the dehydration of methanol to DME is an exothermic reaction, the DME production is favored at low temperature [11].

2.2.2. Direct method

More recently, a direct synthesis method has been developed. This route allows the synthesis of DME directly from syngas: the methanol production production and dehydration occurs in a single reactor and using bi-functional catalysts. The reaction involved in this process as well as the flowsheet of the DME production plant is presented in the section of direct synthesis method [11].

2.3. Method to Improve Increasing Yield of Dimethyl Ether Production

In chemical manufacturing, achieving high conversion is a fundamental requirement, as it directly influences product yield, process efficiency, and economic performance. This principle is particularly relevant to the industrial synthesis of Dimethyl Ether (DME), where reaction conditions must be carefully managed to maintain optimal catalytic activity and equilibrium behavior [5]. As DME continues to emerge as an important clean synthetic fuel and platform chemical within the energy transition, improving production efficiency becomes increasingly essential. Conventional routes remain limited by heat management, equilibrium constraints, and separation demands, motivating the adoption of optimized technologies [12]. For reactions with relatively mild exothermicity, including certain stages within DME synthesis, maintaining proper temperature regulation is essential to ensure catalyst stability and consistent reaction performance. In such systems, the use of intercoolers between adiabatic reaction stages becomes an important strategy to moderate temperature rise, thereby sustaining favorable conditions for achieving optimal conversion and selectivity in DME production [13].

Modifications were conducted in the dimethyl ether production process to achieve a higher yield level. The improvement is carried out by placing an intercooler between the series reactors. This unit substitutes the previous cooling system to create more favourable reaction conditions and consequently increase the overall yield.

3. Results and Discussion

3.1. Comparison Between Basic and Modified Process

The simulation of dimethyl ether (DME) production via methanol dehydration, for both the basic and modified configurations, is illustrated in Figures 1–3. The basic process flow diagram (PFD) is shown in Figure 1, with its corresponding Aspen HYSYS flowsheet presented in Figure 2. In

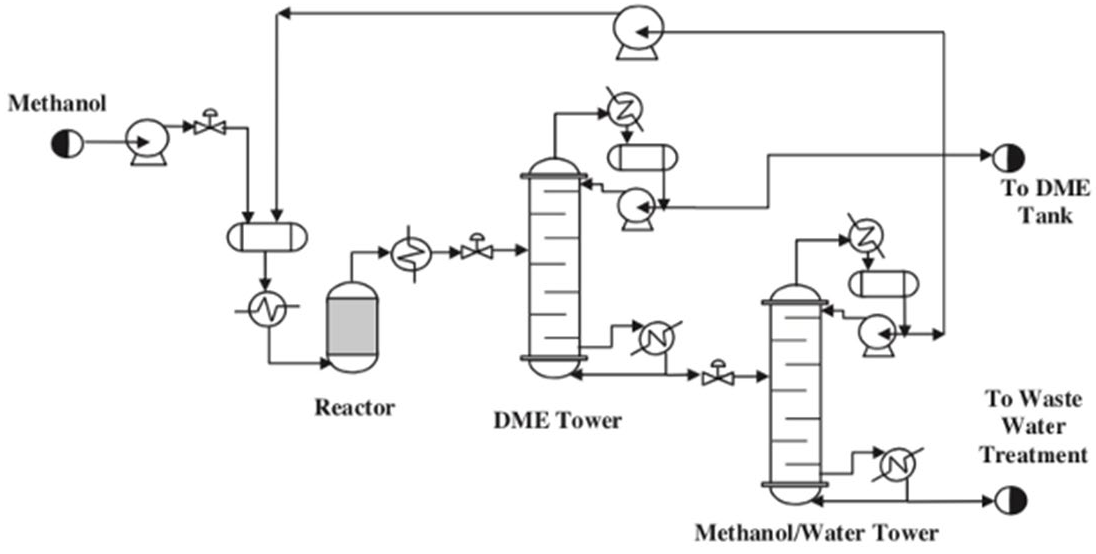

Figure 1. Process Flow Diagram (PFD) of basic (unmodified) process.

this configuration, a single reactor is employed, where methanol undergoes catalytic dehydration to form DME. The modified Aspen HYSYS simulation is shown in Figure 3. In this enhanced configuration, two reactors are arranged in series, with an intercooler installed between them. After methanol reacts in the first reactor (R-1), the outlet stream is cooled in the intercooler before entering the second reactor (R-2). This modification creates more favourable reaction conditions and leads to higher methanol conversion and increased DME yield.

3.2. Process Modification: Improving Yield of Dimethyl Ether

The modification process to improve the yield of dimethyl ether production can be carried out in various ways. In this study, placing an intercooler between two series reactors is used to improve the yield of dimethyl ether production. The modification of the dimethyl ether production process by placing an intercooler between two reactors in series is an engineering approach commonly used to control the heat generated by the exothermic reaction and to increase per-pass conversion. In the methanol dehydration reaction to DME, the significant release of heat can create local hot spots that reduce selectivity, making inter-bed temperature control critically important. In a two-reactor configuration, the first reactor functions to achieve an initial partial conversion by consuming a substantial portion of the more reactive feed while releasing heat that must subsequently be managed. The intercooler installed after the first reactor lowers the reactor effluent temperature, enabling partial condensation of liquid products such as water and unreacted methanol, as well as facilitating inter-stage phase separation. The addition of an intercooler is an effective strategy to shift the reaction equilibrium toward DME formation through the in-situ removal of water. With a cooler stream and reduced water concentration, the second reactor can then operate under more favorable conditions to continue the conversion of the remaining methanol with improved selectivity and significantly lower hotspot risk. This modification increases the per-pass conversion and DME yield while reducing the need for gas recycle and the energy load for separation, as interstage cooling enables heat recovery and energy-saving integration that collectively reduce overall operating costs.

In the modification of the dimethyl ether production process, an intercooler (C-101) was added between two reactors arranged in series (R-100 and R-101). The reason for placing the intercooler is to lower the temperature of the

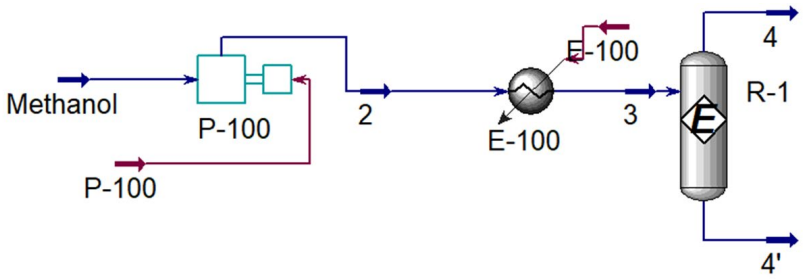

Figure 2. Process simuolation of unmodified process.

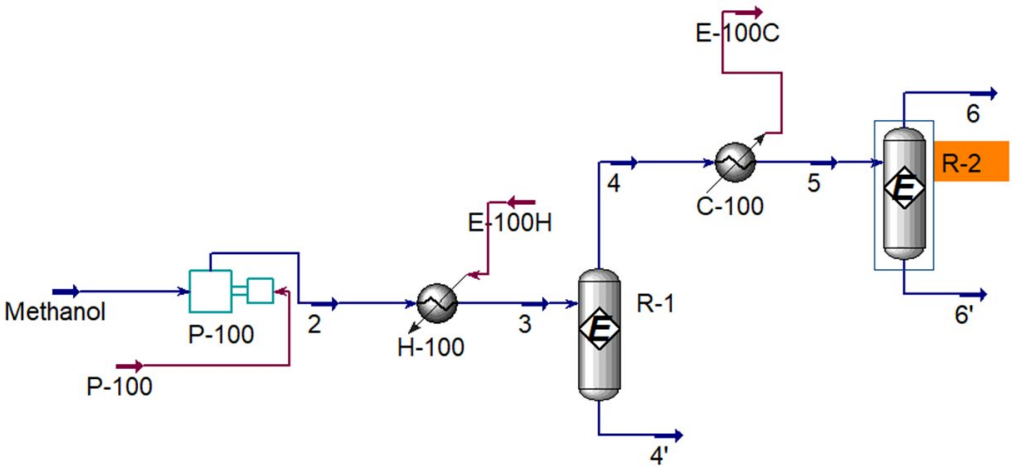

Figure 3. Process simulation of modified process.

outflow from the first reactor (R-100), which shifts the reaction towards DME formation, so that the second reactor (R-101) produces higher conversion with less work.

3.3. Yield Analysis between Unmodified and Modified Processes

After running the simulation, the improvement in product yield becomes clearly evident. The modified configuration achieves a higher overall conversion of methanol, which directly increases the production of dimethyl ether compared to the basic system. This enhancement can be quantified by comparing the molar flow rates of DME in both cases. The yield data obtained from the simulation are summarized in Table 1. The results indicate that the modified process delivers a substantial increase in yield, demonstrating its superior performance relative to the unmodified flowsheet. In addition to producing more DME, the improved configuration also optimizes the reaction conditions, leading to a more efficient utilization of the reactor system.

4. Conclusion

Modifications were implemented in the dimethyl ether (DME) production process to enhance yield and overall process performance. The primary improvement involved installing an intercooler between the series reactors, replacing the original cooling arrangement. By enabling better temperature control and gradual equilibrium shifting, this design effectively overcomes thermodynamic limitations and the temperature spikes caused by the reaction's exothermic nature. The intercooler lowers the outlet temperature from the first reactor, allowing partial condensation and in situ water removal, which creates more favorable conditions for the second reactor to continue the conversion process with improved selectivity. This adjustment establishes more favourable reaction temperatures, mitigates equilibrium limitations, and boosts catalytic activity, thereby increasing the efficiency of methanol-to-DME conversion. Consequently, the overall DME yield rose markedly from 40.87% (4936.9973 kg/h) in the original system to 62.29% (5211.4485 kg/h) in the modified configuration. These results demonstrate that targeted process adjustments even at the level of thermal management can significantly influence conversion and product formation in DME synthesis. Nonetheless, further investigation is required to assess the long-term implications of these modifications, particularly with respect to catalyst stability, energy consumption, and environmental impact, as sustainability considerations continue to gain importance in modern chemical processing.

Table 1. Comparison process without modification and with modification.

Process	DME Flow (kg/h)	DME Yield (%)
Without modification	4936.9973	40.87
With modification	5211.4485	62.29

CRedit Author Statement

Author Contributions: S.A. Nurfiana: Conceptualization, Investigation, Methodology, Software, Data Analysis, Validation, Visualization, Supervision, Project administration, Writing Original Draft, Writing Review & Editing; F.Z. Shofa: Conceptualization, Software, Data Analysis, Writing Original Draft, Writing Review & Editing, Resources, Validation; L. Larasati: Conceptualization, Software, Data Analysis, Writing Original Draft, Writing Review & Editing, Resources, Validation; Y. Dayita: Conceptualization, Methodology, Data Analysis, Validation, Writing Original Draft, Writing Review & Editing; S. Cahyaningsih: Conceptualization, Resources, Data Analysis, Writing Original Draft, Writing Review & Editing, Validation. All authors have read and agreed to the published version of the manuscript.

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