

Improving Energy and Economic Efficiency in Dimethyl Ether Production through Heat Duty Reduction in a Two-Stage Methanol Dehydration Process

Faza Ryviansyah Nurdin^{1*}, Hasnaa Annisafitri¹, Jonathan Hasian¹, Risya Prasetya Muzaki¹, Shafa Novian Andrea Towidjojo²

¹Department of Chemical Engineering, Faculty of Engineering, Universitas Diponegoro, Semarang, Indonesia.

²Department Chemical Engineering, Faculty of Engineering, Universitas Negeri Semarang, Indonesia.

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Abstract

This study investigates the optimization of a two-step dimethyl ether (DME) production process via methanol dehydration, with a focus on enhancing thermal and economic performance through strategic heat integration. A modified configuration was developed by redirecting residual heat from coolers to pump inlets and transferring thermal energy from the condenser of the secondary distillation column to the reboiler of the primary column. These internal heat recovery strategies significantly reduced external utility demand without compromising product purity or plant throughput. Simulation results demonstrate a reduction in total energy consumption from 4,466,363.8 kJ/h to 3,211,110 kJ/h, equivalent to a 31.03% decrease in thermal energy requirement. In parallel, the annual utility cost was reduced by 58.15%, and the annual operating cost decreased by 12.77%, yielding total savings of \$407,304 per year. Importantly, the modified process maintained a DME purity exceeding 99% and preserved the original production capacity of 50,000 tons per year, confirming the feasibility of these improvements without compromising performance targets. Overall, the proposed retrofit offers a more energy-efficient and cost-effective pathway for industrial-scale DME production, serving as a model for sustainable process design in energy-intensive chemical systems.

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Keywords: Dimethyl ether (DME); Methanol dehydration; Heat integration; Energy efficiency; Process optimization

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1. Introduction

As a clean-burning fuel and useful chemical building block, dimethyl ether (DME) stands out as a leading candidate for sustainable energy solutions. Given its adaptability and wide-ranging uses, dimethyl ether (DME) is drawing more attention in response to global pollution and energy security issues [1]. DME can be synthesized from syngas, a mixture derived from natural gas, coal, or biomass. Industry projections estimated a 15.67% market expansion for DME in 2020, with total production expected to hit 20

million metric tons worldwide [2]. Dimethyl ether (DME) is a clean-burning, liquefiable C₁ compound used as an LPG alternative, aerosol propellant, industrial feedstock, and diesel substitute with ultra-low emissions [3]. It also serves as a precursor for chemicals like methyl acetate and olefins, and as a hydrogen carrier for fuel cell applications [4]. Dimethyl ether (DME) is also an efficient, renewable C₁ fuel producible from captured CO₂ and green H₂ via sorption-enhanced synthesis, achieving >90% single-pass conversion while offering a clean alternative to LPG, diesel, or methanol in domestic, transport, and off-grid power applications. It also serves as a low-impact aerosol propellant, refrigerant, chemical intermediate for methyl acetate and

* Corresponding Author.
Email: fazanurdin2735@gmail.com (F.R. Nurdin)

olefins, and functions as a hydrogen carrier for fuel-cell systems [5]. Dimethyl ether (DME) exhibits exceptional properties as a clean fuel alternative. With an oxygen content of approximately 34.8%, it combusts without producing soot—a major advantage over conventional diesel, which faces inherent trade-offs between NO_x and particulate emissions. In addition, DME's favorable physical characteristics, including a boiling point of -25°C and a liquefaction pressure of only 0.5 MPa at ambient conditions, facilitate efficient storage, handling, and distribution within existing LPG infrastructure [6].

Dimethyl ether (DME) can be synthesized by employing either a conventional two-step process, in which methanol is first produced from syngas and subsequently dehydrated over an acidic catalyst, or a single-step direct synthesis that utilizes a bifunctional catalyst within a single reactor. The integrated one-step route provides thermodynamic and kinetic advantages by continuously shifting the equilibrium through in situ methanol removal, thereby improving DME yield and overall process efficiency. In contrast, the single-step method combines methanol synthesis and its dehydration within a single reactor using a bifunctional catalyst [7]. Compared to methanol synthesis catalysts, a wider variety of catalytic systems have been investigated for enhancing methanol-to-DME conversion. These include $\gamma\text{-Al}_2\text{O}_3$, various zeolite structures, ion-exchange resins, aluminophosphates (ALPO), silicoaluminophosphates (SAPO), heteropoly acids (HPAs), Ta-supported Al_2O_3 , polymer-ceramic composite membranes, $\text{NbO}_x/\text{TiO}_2$ composites, and Fe_3O_4 -promoted $\gamma\text{-X-Al}_2\text{O}_3$ systems [2]. Dimethyl ether (DME) can be synthesized in a two-stage process where syngas is converted to methanol over a $\text{CuO-ZnO-Al}_2\text{O}_3$ catalyst at approximately 275°C and 30–70 bar, followed by methanol dehydration using acidic catalysts such as $\gamma\text{-Al}_2\text{O}_3$ or ZSM5. This configuration demonstrates that operating within $240\text{--}290^\circ\text{C}$ and 30–70 bar a range overlapping with 50–100 bar yields high DME selectivity and conversion in industrial-like conditions [8]. In the previous research, the study by Alshbuki *et al.* (2020) employs the conventional two-step DME synthesis method, wherein methanol—sourced from an external plant—is dehydrated over an acid zeolite catalyst in a fixed-bed reactor. The process simulation, carried out using Aspen HYSYS, demonstrates efficient design and thermal integration, supported by the use of heat exchangers and dual distillation columns for separation. With an equilibrium-limited reactor conversion reaching 80%, the process achieves

high DME purity (99.9 mol%) and reflects favorable performance for industrial-scale application. The DME production scheme proposed by Alshbuki [9] provides a complete process flow for direct synthesis from syngas; however, the design lacks any energy integration strategy, resulting in significant thermal energy losses across units such as the condenser, reboiler, and product separation systems. This inefficiency presents a major gap, particularly in the context of industrial feasibility where energy consumption directly affects operational costs. In contrast, our present study introduces a retrofitted configuration incorporating heat recovery through cross-stream integration, reduced cooling loads, and optimized thermal coupling between units. The aim of these modifications is intended to enhance process efficiency by lowering the overall energy demand, specifically by reducing heat duty throughout key thermal operations. As a result, reducing thermal duty not only optimizes energy utilization but also contributes to lowering operational costs associated with heating utilities [10].

2. Methods

2.1 Dimethyl Ether (DME) Production

Referencing from earlier literature approach for DME production from methanol dehydration, Aspen HYSYS v.11 was used for simulation, design, and optimization. The system includes methanol, water, and DME as main components, with trace amounts of CO , CO_2 , CH_4 , H_2 , ethanol, and acetaldehyde. NRTL model was used for the vapor phase, and for liquid phase behavior [9].

The methodology applied in this study is based on process simulation and energy integration techniques using Aspen HYSYS v.11, specifically designed to improve thermal and economic performance in a two-stage methanol dehydration process for dimethyl ether (DME) production. The approach involves retrofitting the base process through internal heat integration, which includes transferring heat from the condenser of the second distillation column to the reboiler of the first column, and repurposing waste heat from coolers to preheat feed streams at pump inlets. Furthermore, the system incorporates recycle loops for methanol and water, contributing to the reduction of external utility consumption.

In this simulation, the modification for optimizing the energy efficiency starts by adding of a pump (P-100) with A 262 kmol/h methanol feed at 25°C and 100 kPa. The raw material is mixed with the recycle stream R coming from the separation by adding a mixer (Mix-100). Then, the heater (E-100), was added after adding pump to

increase the temperature of water and methanol. Adding an equilibrium reactor (ERV-100) aims to separate DME, methanol, and water. The mixture of water, methanol and DME comes out as vapor product and the mixture of water - DME as liquid product. The vapor product contains 54.89 kgmole/h of methanol, water, and DME mixture, while the liquid product contains 214.9 kgmole/h of water and DME mixture. The vapor stream exiting the reactor comprising mixture of DME, methanol, and water is condensed via a cooler (E-101) prior to introduction into the distillation column. A modification in this system involves repurposing the waste heat from the cooler to power the Pump (P-101), enhancing overall energy efficiency. The condensed mixture then enters the distillation column (T-100) to separate DME from methanol and water. The condensed mixture then enters the distillation column (T-100) to separate DME from methanol and water. The distillate produced is DME with a purity of 99.9% and waste of 10.86 kgmole/h methanol – water mixture. The second distillation column (T-101) was added, this aims to separate methanol from water. The bottom product of the first distillation column then enters the second distillation column (T-101). The distillate from the second distillation column is methanol with a purity of 83.6%, while the bottom product produced is 3.443 kmole/h water. The heat released by the condenser in the first distillation column is recycled back to the reboiler in the first distillation column. This aims to save energy used for the heating process. The subsequent modification involves the bottom product (water) from the second distillation column passing through the cooler (E-102). The heat released by the cooler is recycled to the pump (P-100). Meanwhile, the distillate (methanol) is directed to the pump (P-101) to elevate its pressure, enabling it to be recycled and fed back into the mixer. The optimization results in a notable decrease in both the overall heating load and yearly operational expenses, with a 27% improvement in energy efficiency.

2.2 Thermodynamic Study

Catalyst is widely used for methanol synthesis from syngas, typically operating at 260 – 270 °C [11]. Thermodynamic analysis serves two critical purposes: determining the reaction's thermal nature (exothermic or endothermic) through enthalpy change (ΔH) evaluation, Gibbs free energy (ΔG), and establishing reaction reversibility by assessing equilibrium constants (K) [12].

The standard enthalpy change at 298K (ΔH_{298K}^0) for all components involved in the methanol dehydrogenation reaction to dimethyl ether is provided below [13]:

$$\begin{aligned}\Delta H_{298K}^0 \text{ CH}_3\text{OH} &= -201.17 \text{ kJ/mol} \\ \Delta H_{298K}^0 \text{ CH}_3\text{OCH}_3 &= -184.1 \text{ kJ/mol} \\ \Delta H_{298K}^0 \text{ H}_2\text{O} &= -241.8 \text{ kJ/mol} \\ \Delta H_{298K}^0 &= \Delta H_{f, 298K}^0 \text{ product} - \Delta H_{f, 298K}^0 \text{ reactant} \\ &\Rightarrow [-184.1 \text{ kJ/mol} + (-241.8 \text{ kJ/mol})] - [2 \times (-201.17 \text{ kJ/mol})] = -23.56 \text{ kJ/mol}\end{aligned}$$

The negative ΔH confirms the exothermic nature of the reaction, wherein heat is liberated. Elevated operating temperatures adversely affect conversion efficiency; thus, cooling is required to maintain optimal reaction conditions [14].

The ΔG_{298K}^0 for all components involved in the methanol-to-dimethyl ether dehydrogenation reaction is presented below:

$$\begin{aligned}\Delta G_{298K}^0 \text{ CH}_3\text{OH} &= 162.51 \text{ kJ/mol} \\ \Delta G_{298K}^0 \text{ CH}_3\text{OCH}_3 &= -112.93 \\ \Delta G_{298K}^0 \text{ H}_2\text{O} &= -228.6 \text{ kJ/mol} \\ \Delta G_{298K}^0 &= \Delta G_{f, 298K}^0 \text{ product} - \Delta G_{f, 298K}^0 \text{ reactant} \\ &\Rightarrow [-112.9 \text{ kJ/mol} + (-228.6 \text{ kJ/mol})] - [2 \times (-162.51 \text{ kJ/mol})] = -16.48 \text{ kJ/mol}.\end{aligned}$$

The calculated standard Gibbs free energy change at 298 K ($\Delta G_{298}^0 = -16.48 \text{ kJ/mol}$) confirms the spontaneous nature of this reaction, as indicated by the negative value ($\Delta G_{298}^0 < 0$) [15].

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

so that, $K_{298} = 774.331$

At the reaction temperature of 543.15 K, the equilibrium constant (K) is determined through the following equation:

$$\begin{aligned}\ln \frac{K_{543.15}}{K_{298}} &= \frac{\Delta H_{298K}^0}{R} \times \left(\frac{1}{T} - \frac{1}{T_{ref}} \right) \\ \ln \frac{K_{543.15}}{774.331} &= \frac{-23560}{8.314 \frac{\text{J}}{\text{mol.K}}} \times \left(\frac{1}{543.15} - \frac{1}{298} \right) \\ \ln \frac{K_{543.15}}{774.331} &= -4.29201 \\ \text{so that, } K_{543.15} &= 10.6083\end{aligned}$$

At the operating temperature of 270 °C (543.15 K), the reaction equilibrium constant reaches a value of 10.6083, indicating irreversible reaction behavior under these conditions. The standard Gibbs free energy of formation (ΔG_f^0) values for the key components involved in the DME production reaction are presented in Table 1. These thermodynamic data provide the basis for

Table 1. Data ΔG_f^0 for each component at temperature $\Delta G_{f, 298K}^0$ [19].

Compounds	Molecular Formula	$\Delta G_{f, 298K}^0$ (kJ/mol)
Methanol	CH ₃ OH	-162.51
Dimethyl ether	(CH ₃) ₂ O	-112.93
Water	H ₂ O	-228.59

assessing the spontaneity and thermodynamic favorability of the reaction under standard conditions.

3. Result and Discussion

3.1 Comparative Process Flow Reconfiguration for Energy Demand Minimization

In contrast to the baseline setup, the modified process incorporates a systematic internal heat recovery strategy aimed at enhancing thermal efficiency and reducing reliance on external utilities [16]. A key feature of this configuration is the redirection of the outlet stream from the first cooler (E-101) to the suction side of pump P-101, thereby utilizing its residual thermal energy to lower the compression workload [17]. Moreover, thermal energy released from the condenser of the secondary distillation column (T-101) is strategically transferred to drive the reboiler of the primary column (T-100), significantly reducing the need for external heating [18]. Additionally, the effluent from the second cooler (E-102) is routed to the inlet of pump P-100, enabling feed preheating and diminishing thermal duty within the heater section. Collectively, these process modifications

facilitate a higher degree of heat integration, translating to substantial reductions in utility demand and operating costs, while preserving overall process integrity and conversion efficiency. Figures 1 and 2 depict the process flow diagrams (PFDs) adapted from the reference design reported in the literature, representing the conventional dimethyl ether (DME) production pathway via methanol dehydration. These figures serve as the baseline for evaluating process performance and identifying potential areas for improvement. In contrast, Figures 3 and 4 present the modified PFDs developed in this study, which incorporate several design

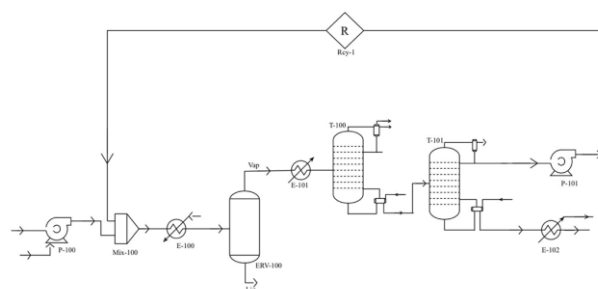


Figure 1. Basic process flow diagram of DME production via methanol dehydration [1].

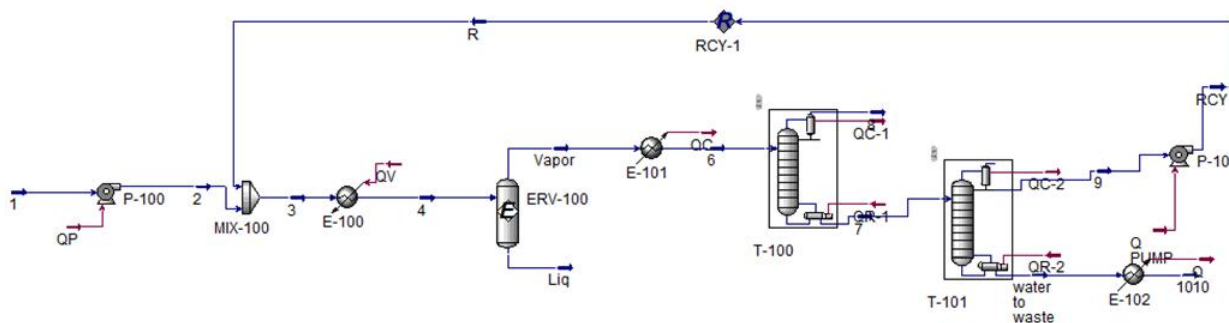


Figure 2. Aspen HYSYS simulation of the basic DME production via methanol dehydration.

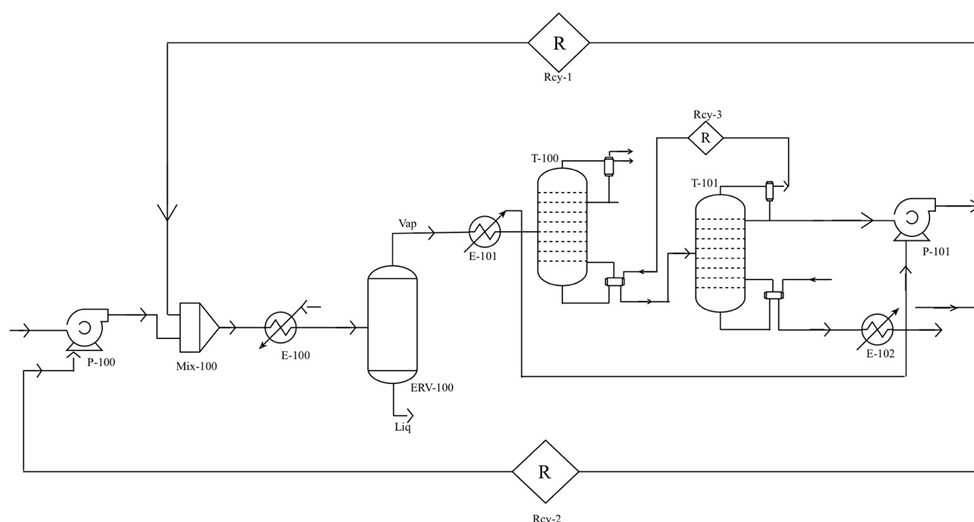


Figure 3. Modified process flow diagram of DME production via methanol dehydration [1].

enhancements aimed at improving energy efficiency, optimizing heat integration, and enhancing overall process reliability.

3.2 Quantitative Assessment of Energy Efficiency in Pre- and Post-Retrofit Configurations

This reconfiguration results in an absolute energy savings of 1.257×10^6 kJ/h, translating to a 31.03% reduction relative to the baseline process. The design improvements are primarily achieved through the elimination of excessive cooling duties and minimization of heat losses. A detailed comparison of energy consumption across key process streams in the pre- and post-retrofit configurations is presented in Table 2, clearly highlighting the impact of the proposed design modifications on overall process energy efficiency and performance. These recycle streams not only reintegrate valuable mass and energy back into the system but also stabilize thermal gradients, reducing the burden on external utility systems. Such a significant enhancement in energy performance positions the modified process as a more sustainable and economically attractive alternative, aligning with global objectives for energy-intensive industries to reduce both

Table 2. Comparison of energy required for pre-retrofit and post-retrofit configurations.

Energy stream	Pre-Retrofit Configurations (kJ/h)	Post-Retrofit Configurations (kJ/h)
QP	1.843e+4	3.078e+4
QV	2.672e+6	-
QC-1	1.619e+5	1.703e+5
QR-1	2.146e+5	-
QC	5.479e+5	5.479e+5
Q PUMP	263.8	-
QR-2	4.079e+5	4.037e+5
QC-2	4.137e+5	4.045e+5
Q-10	3.067e+4	3.043e+4
QH	-	-1.452e+6
QC-3	-	4.045e+5
Total	4,466,363.8	3,211,110

operational expenditure and environmental impact.

3.3 Quantifying Capital and Utilities Cost Reduction through Heat Integration in the Modified DME Process

The cost comparison between the basic and modified DME processes shows a clear reduction in both capital and utilities costs as a result of heat integration improvements. By redirecting heat from the condenser to the reboiler and from the coolers to the pump inlets, the modified process improves energy efficiency and reduces external utility demand. As shown in Tables 3 and 4, the total capital cost and annual utility expenses are both lower in the modified configuration, demonstrating its economic benefit.

4. Conclusion

The implementation of targeted process modifications in the two-step dimethyl ether (DME) production system—specifically, the integration of internal heat recovery between key thermal units—resulted in significant improvements in both energy efficiency and economic performance. The total energy demand of the modified process was reduced by 1.257×10^6 kJ/h, representing a 31.03% decrease relative to the baseline configuration. This improvement is primarily attributed to the reutilization of thermal energy from the condenser to support reboiler duties, as well as from coolers to preheat

Table 3. Utilities cost comparison for pre- and post-retrofit configurations.

Cost Item	Amount of cost (USD/Year)		
	Pre-Retrofit Configurations (USD/Year)	Post-Retrofit Configurations (USD/Year)	Saving (USD / Year)
Electricity	6,290	4,199	2,091
Cooling	56,799	39,195	17,604
Heating	271,507	96,588	174,919
Total	334,596	139,982	194,614

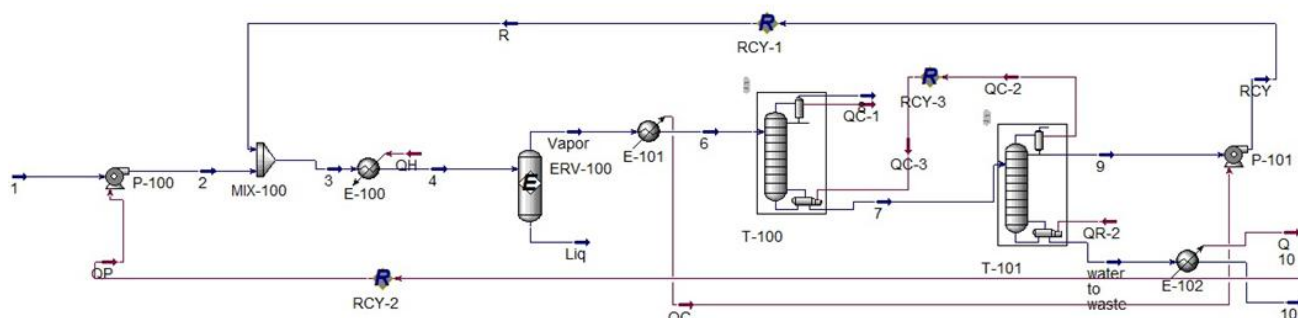


Figure 4. Aspen HYSYS simulation of the modified DME production via methanol dehydration.

pump inlet streams, thereby minimizing the burden on external utility systems. Capital expenditure was also optimized, with the total capital cost reduced by \$2,330, while the annual operating and utility costs decreased by \$210,360 and \$194,614, respectively. These reductions were achieved without compromising the process stability or product purity, confirming that the retrofitted configuration offers a more energy-efficient, cost-effective, and industrially viable alternative to the original design. Energy-efficiency retrofits can reduce consumption and emissions without compromising system performance, offering a cost-effective and scalable solution [20]. Overall, this study highlights the potential of heat integration strategies to advance the sustainability of DME production and serve as a framework for optimizing other energy-intensive chemical processes.

CRedit Author Statement

Authors contributions: F. R. Nurdin led the conceptualization, supervised the overall research process, and contributed to writing and final manuscript revision. H. Annisafitri was responsible for methodology development, data visualization, and simulation validation. J. Hasian conducted the investigation, supported formal analysis, and participated in editing the manuscript. R. P. Muzaki handled software development, process modeling, and assisted in project coordination. S. N. Towidjojo contributed to thermodynamic analysis, wrote the initial draft of the manuscript, and supported the review process. All authors have read and agreed to the published version of the manuscript.

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Table 4. Overall cost comparison for pre- and post-retrofit configurations.

Cost Item	Amount of cost (USD/Year)		
	Pre-Retrofit Configurations (kJ/h)	Post-Retrofit Configurations (kJ/h)	Saving
Total capital cost	3.730.160	3.727.830	2.330
Total operating (cost/year)	1647.260	1.436.900	210.360
Total Raw Material (cost/year)	0	0	0
Total Utilities (cost/year)	334.596	139.982	194.614
Total	5.712.016	5.304.712	407.304

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