

## Design Enhancement of Methanol Purification in Syngas-Based Production: The Role of Additional Distillation and Cooling

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### Abstract

Methanol is an essential industrial chemical with increasing global demand, yet conventional syngas-based production often encounters challenges related to energy efficiency and separation performance. This study seeks to design and evaluate an improved methanol purification process aimed at maximizing yield and purity through advanced heat management and separation strategies. Employing a rigorous process simulation environment and the Peng–Robinson Equation of State (PR-EOS) for thermodynamic modeling, a comparative analysis was conducted between a conventional base case and a modified process configuration. The base case comprised a single cooling unit, a separator, and one distillation column, whereas the modified design incorporated an additional upstream cooler and a secondary distillation column to enhance phase conditioning and recovery. Simulation results indicate that the proposed modifications substantially outperform the conventional design. The base case achieved a methanol purity of 59.26%, while the modified configuration increased purity to 71.07%. This 11.8% improvement demonstrates that multi-stage distillation combined with enhanced cooling effectively reduces vapor-phase losses and improves separation efficiency, offering a more sustainable pathway for industrial methanol production.

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**Keywords:** Methanol Purification; Syngas; Distillation; Cooling system

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### 1. Introduction

Methanol is a versatile and indispensable chemical that plays a pivotal role in the global economy. It serves as a key raw material in the production of plastics, paints, adhesives, and synthetic fibers [1]. Worldwide demand for methanol continues to grow, with a compound annual growth rate (CAGR) of 5.2%. Its consumption and production represent nearly 10% of the global chemical sector. This rising demand is driven both by methanol's broad industrial applications and its emerging potential as a cleaner alternative fuel [2].

The synthesis of methanol from syngas involves two primary stages. First, syngas is

generated from natural gas (methane) [3], where methane reacts with steam or oxygen to produce a mixture of carbon monoxide and hydrogen. In the second stage, this syngas is converted into methanol within a reactor operating under controlled pressure and temperature conditions. The resulting product stream, which contains methanol along with water and dissolved gases, is subsequently subjected to distillation to achieve separation and purification [4].

Previous studies have demonstrated that gas reforming processes, such as steam methane reforming (SMR) and autothermal reforming (ATR), generate high-temperature gases that can be effectively utilized for heating. However, in current systems, the integration of heat exchangers for energy recovery remains under-optimized. As a result, a considerable portion of

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waste heat is released without being efficiently harnessed to lower energy consumption in downstream operations, including feed gas preheating for reforming and the distillation stage [5].

To improve methanol yield in syngas-based production, process modifications must incorporate advanced separation and heat management strategies, such as multi-stage distillation and enhanced cooling systems. The use of a two-stage distillation column enables more efficient separation of methanol from water. Integrating heat exchangers and an additional distillation column has been reported to reduce energy consumption by 58.5% while increasing methanol yield to 99%. Moreover, the adoption of reactive distillation can substantially boost productivity, achieving a 47% increase in methanol output compared to conventional processes [6]. Collectively, these approaches address both thermodynamic and kinetic constraints, ensuring higher yields with reduced energy demand. The overarching objective of these process modifications is to maximize methanol production efficiency while minimizing resource consumption.

## 2. Materials and Methods

### 2.1 Purification Process of Crude Methanol

Crude methanol obtained from synthesis contains water, dissolved gases, higher alcohols, and trace impurities, making purification essential for industrial applications [7]. The process typically begins with flash separation to remove volatile components such as CO and CO<sub>2</sub>. Distillation is then employed, commonly using two columns: the light-ends column removes low-boiling impurities, while the main methanol column separates methanol from water and heavy organics, yielding refined methanol with a purity of approximately 99.85%. For ultra-pure applications, additional rectification or adsorption steps are implemented to eliminate residual contaminants [8]. Despite its effectiveness, distillation is highly energy-intensive, accounting for nearly 20% of total plant energy consumption, and is further complicated by issues such as azeotrope formation and corrosive impurities. Ongoing advancements in energy integration and process control are therefore critical to achieving efficient and sustainable methanol purification [9].

### 2.2 Separation Mechanisms in Methanol Purification

Methanol purification primarily exploits volatility differences, with distillation concentrating methanol in the overhead stream

while water and heavier impurities remain in the bottoms [10]. The process is governed by vapor–liquid equilibrium, and predictive models such as NRTL and UNIQUAC are commonly employed to describe phase behavior and support efficient column design. In cases where azeotropes arise, advanced techniques such as extractive distillation or pressure-swing distillation are utilized to overcome these limitations [11]. To improve energy efficiency, double-effect distillation integrates heat exchange between columns, thereby reducing operating costs while maintaining separation performance [8]. For ultra-pure methanol applications, adsorption and membrane-based technologies, particularly those employing materials like metal–organic frameworks, enable the selective removal of trace contaminants [12].

### 2.3. Simulation Setup

#### 2.3.1. Software and thermodynamic model

The methanol purification process was simulated using Aspen HYSYS V11, with the corresponding process flowsheet shown in Figure 1. This simulation platform enables rigorous mass and energy balance calculations, vapor–liquid equilibrium modeling, and detailed equipment-level performance analysis. The Peng–Robinson Equation of State (PR-EOS) was selected as the sole thermodynamic package to represent all process conditions due to its proven reliability in predicting phase behavior in systems containing methanol, water, and light gases (CO, CO<sub>2</sub>, H<sub>2</sub>), particularly under the elevated pressures characteristic of syngas-based methanol production. By applying a consistent thermodynamic framework across both cooling and distillation stages, the simulation ensures accurate prediction of condensation, vapor–liquid phase splitting, relative volatility, and column separation performance. This consistency provides a robust basis for realistic comparison

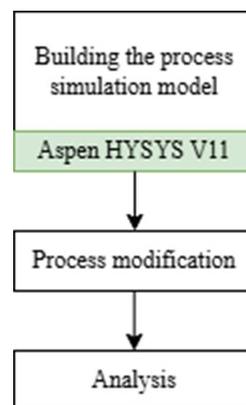


Figure 1. Process integration methodology chart.

between the base and modified methanol purification systems [13].

### 2.3.2. Base case process configuration

The base-case methanol purification flowsheet consists of three main units: (a). Cooling Unit (Cooler-1): Lowers the reactor effluent temperature to initiate partial condensation; (b). Vapor–Liquid Separator: Splits the stream into a non-condensable gas phase and a condensed methanol–water liquid phase; (c). Primary Distillation Column (Column-1): Produces methanol as the overhead product while water is discharged as the bottom product. This configuration replicates a conventional crude methanol purification system and serves as the benchmark for evaluating the effectiveness of purification design enhancements [14].

### 2.3.3. Modified process configuration

To enhance methanol purification efficiency and improve recovery, the modified flowsheet integrates two additional units: (a). Additional Cooling Unit (Cooler-2): Positioned upstream of the separator to achieve deeper cooling, thereby increasing methanol condensation and minimizing vapor-phase losses; (b). Secondary Distillation Column (Column-2): Designed to recover methanol from light-end-rich streams or overhead vapors, providing additional equilibrium stages and improving overall product purity. This enhanced configuration enables a direct and realistic performance comparison with the base case under identical feed conditions.

### 2.3.4. Mass balance and purity calculation

Mass balances for all process streams were automatically solved using Aspen HYSYS convergence algorithms. The purity of methanol in the final product was determined as the mass fraction of methanol relative to the total product mass flow rate, expressed as:

$$\text{Methanol Purity (\%)} = \frac{m_{\text{methanol-product}}}{m_{\text{total-product}}} \times 100\% \quad (1)$$

The purity results from both the base and modified configurations were then compared to quantify the improvements achieved through the

incorporation of additional cooling and distillation stages [15].

### 2.3.5. Energy analysis method

Energy consumption for each cooling and distillation unit, including cooling duties, condenser duties, and reboiler duties, was obtained directly from the Aspen HYSYS V11 simulation results. These values were compared between the base and modified methanol purification configurations to quantify overall utility requirements and evaluate potential energy savings. The analysis emphasized reductions in reboiler duty, condenser duty, and total cooling load, thereby underscoring the operational advantages of the enhanced design [10].

### 2.3.6. Modeling assumptions

The simulation was developed under a unified set of assumptions to ensure reliability and comparability between the base and modified methanol purification systems: (a). Operating Conditions: All units were modeled under steady-state operation, with nochemical reactions occurring during purification; (b). Equipment and Hydraulics: Equipment and pipelines were assumed to be adiabatic, with pressure drops across all units considered negligible; (c). Thermodynamics: Vapor–liquid equilibrium was assumed to be fully established in separators and distillation stages. Physical property data were obtained directly from the AspenTech database using the Peng–Robinson EOS framework; (d). Operational Integrity: No fouling, degradation, or process disturbances were incorporated into the model. These assumptions align with standard industrial simulation practices and provide a consistent basis for evaluating modifications to methanol purification system design [15].

## 3. Results and Discussion

### 3.1. Process Description

The concept described in the literature forms the basis of the methanol production process [14]. An industrial methanol plant based on syngas is illustrated in Figure 2. The simulation model was developed using Microsoft Visio, with the reactor

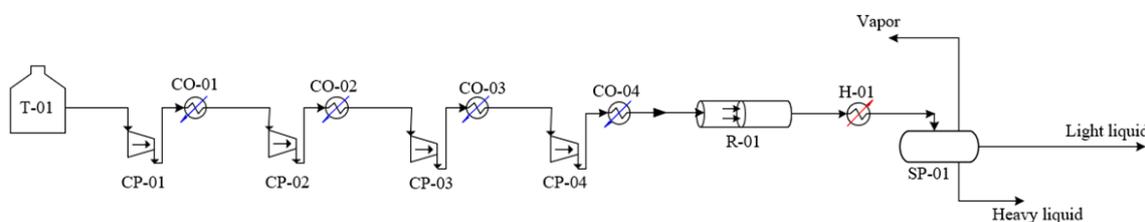
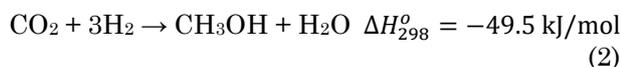


Figure 2. Process Flow Diagram (PFD) of basic methanol production.

represented as a plug flow reactor operating at 220.1 °C and 98.69 atm. To accurately account for multiphase behavior, the Peng–Robinson thermodynamic model was selected, given its reliability in predicting phase equilibria in systems containing methanol, water, and light gases. The chemical reactions governing this process are presented in Equation (2).



The primary reaction involves the generation of hydrogen and carbon monoxide through the interaction of methanol with water, a process commonly referred to as steam reforming. At the operating temperature, the rates of side reactions are assumed to be negligible. Consequently, the reactor configuration does not incorporate these secondary pathways [16]. As a result, the product stream consists predominantly of hydrogen and carbon monoxide, with minor amounts of unreacted methane and water vapor.

The process configuration includes a compressor, cooler, reactor, and flash drum separator. Among these, the reactor and flash drum separator play a critical role in driving the methane reaction and separating the stream into gas, liquid, and solid phases. The reactor is modeled as a plug flow reactor, selected for its efficiency in promoting methane-based reactions within the gas phase. Prior to reaction, operating conditions are adjusted through pretreatment using heaters or coolers to maintain optimal temperature profiles. The resulting product stream is subsequently directed to purification units, where separation techniques such as absorption and distillation are applied to remove residual components. This yields a product composition primarily consisting of hydrogen and carbon monoxide, with minor traces of unreacted methanol and water vapor.

In summary, methanol production involves the conversion of syngas components in a plug flow reactor, where carbon monoxide or carbon dioxide reacts with hydrogen to yield methanol and water. The kinetic equation intended for use in the simulation is as follow:

$$k'_{ps,A} = (4.36 \pm 0.25) \times 10^2 \times \exp\left(\frac{-65,200 \pm 200}{RT}\right) \quad (3)$$

$$k'_{ps,B} = (7.31 \pm 4.90) \times 10^8 \times \exp\left(\frac{-123,400 \pm 1600}{RT}\right) \quad (4)$$

$$k'_{ps,C} = (2.69 \pm 0.14) \times 10^7 \times \exp\left(\frac{-109,900 \pm 200}{RT}\right) \quad (5)$$

The resulting product stream is then directed to separation units, such as flash drum

separators and absorbers, to remove water and unreacted gases. Purification is subsequently carried out through multistage processes, producing a methanol-rich stream suitable for downstream applications. The detailed methodology of methane synthesis is presented in the following chapter [17].

### 3.2. Process Simulation

The process flow diagram depicts a syngas-to-methanol production system simulated in Aspen HYSYS V11, employing the Peng–Robinson equation of state to ensure accurate prediction of phase behavior. Aspen HYSYS simulation model for basic (unmodified) methanol production process is depicted in Figure 3 and Table 1. The process begins with a mixed syngas feed entering the first compression stage (CP-1), where the pressure rises from approximately 1 atm to 3 atm and the temperature increases to 158.7 °C. Subsequent compression stages (CP-2, CP-3, and CP-4) further elevate the pressure to about 98.69 atm and the temperature to 369.8 °C, conditioning the feed for methanol synthesis. The compressed stream then enters a plug flow reactor operating under high pressure ( $\approx 98.69$  atm) and elevated temperature ( $\approx 369.8$  °C), where carbon monoxide reacts with hydrogen to produce methanol. The reactor effluent is subsequently cooled and pressure-adjusted before passing into a flash drum, which separates the vapor and liquid phases. The vapor fraction consists primarily of unreacted syngas, while the liquid fraction contains crude methanol along with water and trace impurities.

Overall, the methanol production process in this configuration is not fully optimized for sustainability, as unreacted syngas components and by-products are discharged without recovery or recycling. Following the reaction, the outlet stream is first cooled to lower its temperature before entering the flash drum for vapor–liquid separation. The vapor fraction consists mainly of unreacted gases, while the liquid fraction contains crude methanol mixed with water and trace impurities. To achieve higher product purity, additional distillation columns are required. The first column removes light gases such as CO<sub>2</sub> and residual syngas, while subsequent columns separate methanol from water and heavier components, ultimately producing high-purity methanol. Incorporating deeper cooling and extra distillation stages enhances separation efficiency, minimizes waste, and aligns the process with sustainable design principles. To advance a methanol purification design aligned with sustainable principles, a process modification was implemented, as illustrated in Figure 4 and Table 2.

The modified methanol process design initially follows the same sequence of steps as the base-case system. However, the key distinctions and innovations lie in the approaches to separation, purification, and heat transfer. These enhancements introduce advanced unit operations and integration strategies that improve efficiency, reduce energy consumption, and deliver higher product purity compared to the conventional configuration. In the modified

design illustrated in Figure 4, a cooler (E-101) is installed immediately downstream of the reactor to lower the outlet temperature, thereby establishing optimal conditions for subsequent separation. The cooled stream is then directed to a distillation column (T-101), where methanol is separated from water and heavier components based on differences in boiling points. The overhead stream delivers high-purity methanol, while heavier residues are discharged through the

Table 1. Mass and energy balances of the basic process for methanol production of Figure 3.

Material Streams									
		mixed feed	CP_1	compressed_1	CP_2	compressed_2	CP_3	compressed_3	
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
Temperature	C	24.85	158.7	150.1	331.5	150.1	331.7	150.1	
Pressure	atm	0.9998	2.999	3.000	9.001	9.000	27.00	27.00	
Molar Flow	kgmole/h	4.000	4.000	4.000	4.000	4.000	4.000	4.000	
Mass Flow	kg/h	50.06	50.06	50.06	50.06	50.06	50.06	50.06	
Liquid Volume Flow	m3/h	0.1399	0.1399	0.1399	0.1399	0.1399	0.1399	0.1399	
Heat Flow	kJ/h	-3.938e+005	-3.770e+005	-3.781e+005	-3.542e+005	-3.781e+005	-3.542e+005	-3.782e+005	
		CP_4	reactant	outlet'	outlet''	vapour	Light liquid	Heavy liquid	
Vapour Fraction		1.0000	1.0000	1.0000	0.1146	1.0000	0.0000	0.0000	
Temperature	C	369.8	220.1	701.5	30.05	30.05	30.05	30.05	
Pressure	atm	98.69	98.69	98.69	98.69	98.69	98.69	98.69	
Molar Flow	kgmole/h	4.000	4.000	2.148	2.148	0.2462	1.902	0.0000	
Mass Flow	kg/h	50.06	50.06	50.06	50.06	1.668	48.39	0.0000	
Liquid Volume Flow	m3/h	0.1399	0.1399	6.437e-002	6.437e-002	7.785e-003	5.659e-002	0.0000	
Heat Flow	kJ/h	-3.490e+005	-3.693e+005	-3.693e+005	-5.197e+005	-1.096e+004	-5.087e+005	0.0000	

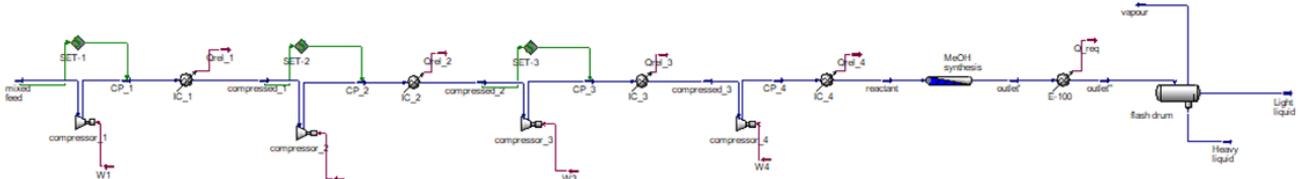


Figure 3. Aspen HYSYS simulation model for basic (unmodified) methanol production process.

Table 2. Mass and energy balances of the modified process for methanol production.

Material Streams								
		mixed feed-2	CP_1-2	compressed_1-2	CP_2-2	compressed_2-2	CP_3-2	compressed_3-2
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
Temperature	C	24.85	158.7	150.1	331.5	150.1	331.7	150.1
Pressure	atm	0.9998	2.999	3.000	9.001	9.000	27.00	27.00
Molar Flow	kgmole/h	4.000	4.000	4.000	4.000	4.000	4.000	4.000
Mass Flow	kg/h	50.06	50.06	50.06	50.06	50.06	50.06	50.06
Liquid Volume Flow	m3/h	0.1399	0.1399	0.1399	0.1399	0.1399	0.1399	0.1399
Heat Flow	kJ/h	-3.938e+005	-3.770e+005	-3.781e+005	-3.542e+005	-3.781e+005	-3.542e+005	-3.782e+005
		CP_4-2	reactant-2	outlet'-2	OUTLET"-2	Methanol Product	Ovhd Liq outlet	Bottoms Liq outlet
Vapour Fraction		1.0000	1.0000	1.0000	0.1204	0.2603	0.1317	0.0000
Temperature	C	369.8	220.1	701.5	100.0	50.00	-127.2	99.96
Pressure	atm	98.69	98.69	98.69	98.69	1.000	1.000	1.000
Molar Flow	kgmole/h	4.000	4.000	2.148	2.148	1.682	1.682	0.4624
Mass Flow	kg/h	50.06	50.06	50.06	50.06	41.72	41.72	8.330
Liquid Volume Flow	m3/h	0.1399	0.1399	6.437e-002	6.437e-002	5.591e-002	5.591e-002	8.347e-003
Heat Flow	kJ/h	-3.490e+005	-3.693e+005	-3.693e+005	-5.055e+005	-3.778e+005	-4.115e+005	-1.296e+005

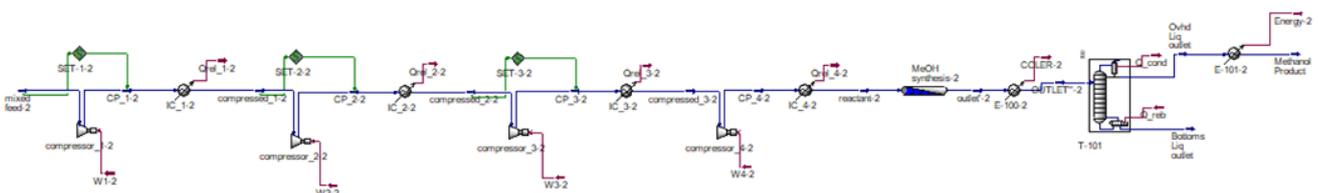


Figure 4. Aspen HYSYS simulation model for the modified methanol production process.

bottom outlet. By incorporating this additional cooler and distillation column, the modified configuration improves phase conditioning, enhances separation efficiency, and achieves higher methanol yield and purity compared to the base case. A detailed comparison of product quality between the base and modified designs are presented in the following section.

### 3.3. Purity Analysis

The quality of methanol products serves as an indicator for both the factory and the overall quality of the products manufactured. A higher level of purity in the product corresponds to superior quality in both the product itself and the factory [18]. To determine the percentage purity in the two simulated processes, calculations are conducted using the Equation (1). The masses of the methanol product and the total product mass were obtained from Aspen HYSYS V11 data. The data for the total product mass in the base process design is interpreted in Table 3.

Using the simulation data, the purity of methanol in the base process system can be calculated as 59.26%. Based on these calculations, the methanol produced in the base process system is estimated to have a purity of 59.26%. For comparison, the purity of methanol in the modified process configuration was determined using the same calculation method. The corresponding mass data for methanol products obtained from the modified process are presented in Table 4. Using the simulation data, the purity of methanol in the modified process system can be calculated as 71.07%. The composition of the product stream, expressed in terms of mass fractions, is presented in Table 5.

A comparison of methanol purity between the base and modified process systems is

Table 3. Composition of basic process system product.

Composition	Mass flow (kg/hour)
Carbon dioxide (CO <sub>2</sub> )	3.2645
Water (H <sub>2</sub> O)	16.6788
Hydrogen (H <sub>2</sub> )	0.4486
Methanol	29.6652
Total product	50.06

Table 4. Composition of modified process system product.

Composition	Mass flow (kg/hour)
Carbon dioxide (CO <sub>2</sub> )	3.2645
Water (H <sub>2</sub> O)	8.3497
Hydrogen (H <sub>2</sub> )	0.4405
Methanol	29.6637
Total product	41.72

presented in Table 6. Based on the purity data, a clear distinction can be observed between the base and modified methanol production systems. The modified process achieves a product purity of 71.07%, which is significantly higher than the 59.26% obtained in the base configuration. This corresponds to a deviation of approximately 11.8%, highlighting the effectiveness of the process modifications in enhancing methanol quality and overall separation efficiency.

### 4. Conclusion

This study clearly demonstrates the successful enhancement of methanol purification in syngas-based production through targeted process modifications. The integration of an additional cooling unit and a secondary distillation column was designed to optimize phase conditioning and improve separation efficiency compared to the conventional single-column base case. Comparative analysis confirmed that the modified configuration substantially improved product quality, achieving a methanol purity of 71.07%, in contrast to 59.26% in the base system. This notable increase of approximately 11.8% highlights the effectiveness of multi-stage distillation combined with enhanced upstream cooling in reducing impurities and maximizing methanol recovery. Overall, the proposed design provides a more efficient, sustainable, and higher-quality approach for industrial methanol production.

### Credit Author Statement

Author Contributions: A. Gracelly: Investigation, Data Curation, Supervision. J. A. L. Sinuraya: Investigation, Formal Analysis, Data Curation. L. A. Y. Talentina: Conceptualization,

Table 5. Composition of modified process system product.

Composition	Mass fraction
Carbon dioxide (CO <sub>2</sub> )	0.0783
Water (H <sub>2</sub> O)	0.2001
Hydrogen (H <sub>2</sub> )	0.0106
Methanol	0.7110
Total	1.000

Table 6. Comparison of methanol purity before and after process modification.

Purity of methanol basic process system production (%)	Purity of methanol production with modification process (%)
59.26	71.07
Residual	11.8

Methodology, Formal Analysis, Writing – Original Draft. M. J. Gandy: Software, Validation, Formal Analysis. R. O. A. Arnata: Resources, Project Administration, Investigation. S. R. Ilaiah: Visualization, Writing – Review & Editing. All authors have read and agreed to the published version of the manuscript.

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