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Techno-Economic Evaluation of an Optimized Process for Solid Sodium Methoxide Production from Methanol and Sodium Hydroxide

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ABSTRACT

Sodium methoxide is commercially available in both solid and liquid forms in global markets. Its liquid form, typically marketed as a 30 wt.% solution in methanol, has gained the dominant market share in recent years due to the significant growth of biodiesel production. Nevertheless, solid sodium methoxide, owing to its wide range of applications in pharmaceutical industries and chemical synthesis, remains of considerable industrial importance, and the development of its commercial production requires comprehensive techno-economic assessments. In this study, an integrated process configuration consisting of reactive distillation, distillation, and spray drying was designed, simulated, and optimized for the production of solid sodium methoxide from methanol and sodium hydroxide solution. Process simulation was carried out using ASPEN Plus software, and mass and energy balances of the individual units were determined. The optimization involved adjusting key operating parameters, including drying-gas conditions in the solidification unit and the number of theoretical stages and reflux ratio of the distillation columns, to minimize energy consumption while meeting the product water-content specification. Subsequently, a techno-economic assessment was performed using the Aspen Process Economic Analyzer for a total plant capacity of 15 $kt.y^{-1}$ of sodium methoxide products, comprising 10 $kt.y^{-1}$ of solid sodium methoxide produced in the spray-drying unit and 5 $kt.y^{-1}$ of a 30 wt.% sodium methoxide methanol solution as a liquid product. The results of the economic analysis demonstrated that the proposed process is economically viable, with an internal rate of return (IRR) of 175% and a payback period of 1.58 years for the specified capacities. These economic indicators are based on conceptual design assumptions, including 100% production capacity after commissioning, a short EPC implementation period of 21 weeks, and the assumed product selling price and raw material costs. The findings of this study indicate that the production of solid sodium methoxide from methanol can be considered an attractive option for the development of the methanol value chain.

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1. Introduction

Sodium methoxide is one of the key chemical compounds with extensive applications in pharmaceutical industries, biodiesel production, and organic synthesis ([1], [2]). Owing to its strong basicity and high catalytic activity, this compound is widely used in esterification and transesterification reactions and plays a significant role in the development of downstream industries [3].

In addition to its application as a catalyst in organic synthesis, sodium methoxide is also utilized as an intermediate in the production of pharmaceuticals, agrochemicals, and industrial additives [4]. In recent years, the growing demand for biofuels has led to a substantial increase in the consumption of sodium methoxide as a catalyst in biodiesel production processes, where it is typically employed as a 25–30 wt.% solution in methanol [5].

Considering the development of pharmaceutical industries and the increasing focus on renewable energy in Iran, the demand for sustainable and economically viable production of sodium methoxide has been steadily rising. Therefore, the investigation of sodium methoxide production processes from both technical and economic perspectives particularly within the framework of the methanol value chain is of great importance.

An analysis of national sodium methoxide import statistics from 1394 to 1402, based on data from the Ministry of Industry, Mine and Trade (Fig. 1), indicates an increasing demand trend in domestic industries. The import volume of this product increased from less than 0.5 kt in 2014 to more than 1.3 kt in 2024, while its import value rose from approximately USD 1.2 million to nearly USD 3.7 million. This upward trend highlights the significant dependence of the domestic market on imports and the existence of sustained demand for this chemical. The steadily rising import volume and value shown in Fig. 1 indicate a growing domestic market that is currently largely dependent on imports, representing a direct opportunity for import substitution and domestic value creation, the central economic motivation for this study. Consequently, investment in domestic sodium methoxide production could reduce import dependency, result in foreign exchange savings, and create added value within the country.

At the global level, various research reports indicate that the sodium methoxide market is experiencing growth with a compound annual growth rate (CAGR) ranging from 3.8% to 8.8%, with an average estimated at approximately 5.3%. In terms of product type, solid sodium methoxide accounts for about 60% of the global market [6], mainly due to its extensive applications in pharmaceutical industries and organic synthesis, whereas the liquid form particularly in biodiesel production has been experiencing a faster growth rate. It is anticipated that in the coming years, both solid and liquid forms will play complementary roles in the global market.

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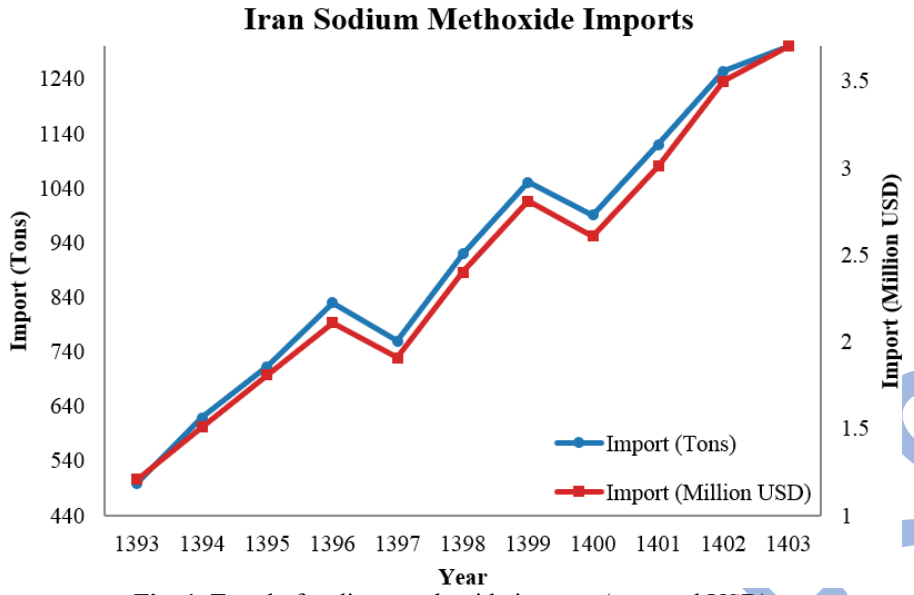


Fig. 1. Trend of sodium methoxide imports (tons and USD).

1.1. Methods for sodium methoxide production

According to the literature, four main routes for sodium methoxide production have been reported based on the type of sodium-containing feedstock: the use of sodium amalgam [7], metallic sodium [8], sodium hydroxide [9], and sodium acetate [10]. The sodium amalgam based method involves the reaction of amalgam with methanol vapor in packed columns. Despite the ease of methanol recovery, its industrial application has been increasingly restricted in recent years due to environmental and safety concerns associated with mercury. associated with mercury, with all mercury-based chlor-alkali capacity in the EU required to convert to alternative technologies by 2020.

The metallic sodium route involves the highly exothermic reaction of molten sodium with methanol, which requires strict temperature control and careful safety management due to hydrogen evolution. due to hydrogen evolution; producing metallic sodium via molten-salt electrolysis also requires substantially more specific energy (~10 MWh per tonne of Na) than the 50 wt.% NaOH solution used in the present route (~4 MWh per tonne) [3]. The sodium hydroxide–based pathway consists of the reaction of excess methanol with an aqueous NaOH solution in reactive distillation columns and is widely employed for the production of commercial sodium methoxide solutions; however, the presence of water can adversely affect the reaction conversion. From an environmental standpoint, this route generates a single aqueous waste stream that, if controlled below 0.1 wt.% residual methanol, can generally be classified as nonhazardous, avoiding the mercury- and hydrogen-handling burdens of the alternative routes described above.

Finally, more recent approaches, such as electrodialysis from sodium acetate, have also been reported. Despite their conceptual attractiveness, these methods have found limited industrial application due to process complexity and high capital investment requirements. In particular, the sodium hydroxide-based process was selected due to the higher safety level associated with handling NaOH compared with metallic sodium, the wide availability and relatively low cost of the raw material, and the simplicity of process implementation at industrial scale. These advantages make the NaOH route a suitable option for the development of a commercially feasible sodium methoxide production process. To assess its industrial feasibility, a chemical plant comprising synthesis, separation, and solidification stages was rigorously modeled and evaluated from both technical and economic perspectives.

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1.2. Proposed industrial configurations for sodium methoxide production

In the design of an industrial sodium methoxide production process, the selection of appropriate equipment in the three main sections reaction, separation, and solidification plays a critical role in determining product quality, methanol recovery, and overall process efficiency. Accordingly, as summarized in Table 1, several proposed industrial configurations are presented, incorporating combinations of conventional and advanced equipment. These configurations enable a comprehensive techno-economic assessment (TEA) of different process pathways. Techno-economic assessment has become an essential tool for evaluating the industrial feasibility of emerging chemical processes. By integrating process simulation with economic analysis, TEA enables the systematic evaluation of capital investment, operating costs, profitability, and the economic impact of alternative process configurations. Recent studies have highlighted the importance of combining process simulation and techno-economic assessment during the early stages of process development to support technology selection, identify cost drivers, and guide process optimization toward economically viable and sustainable industrial implementation ([11], [12], [13]).

Table 1. Proposed industrial configurations for sodium methoxide production.

Reaction	Purification	Separation (Methanol)	Separation (NaOCH3)
Reactive distillation	-	Distillation	dryer
		Pervaporation Membrane	
Reactor	Distillation	Distillation	dryer
		Pervaporation Membrane	
Note: "–" indicates in-situ separation of $NaOCH_3$ within the reactive distillation column.			

The reaction between methanol and sodium hydroxide for the production of sodium methoxide can be carried out in two types of reaction units. In the first approach, a conventional reactor is employed, where the reaction takes place independently and the reaction products are subsequently directed to downstream separation units. In the second approach, a reactive distillation column is employed, where reaction and separation occur simultaneously within a single process unit [14]. Recent studies and reviews have demonstrated that reactive distillation remains an active process-intensification strategy, with significant advances reported in feasibility assessment [15], process controllability [16] and economic evaluation [3]. These studies have highlighted that integrating reaction and separation in a single column can reduce the number of process units while improving reaction conversion, process efficiency, and energy utilization. Therefore, the selection of reactive distillation as a route for sodium methoxide production is supported by recent advances reported in the scientific literature.

Following the reaction step, the separation process is conducted in two stages. In the first stage, the objective is to separate sodium methoxide from the liquid reaction phase consisting of methanol and water. It should be noted that the allowable water content in the sodium methoxide solution must not exceed 0.1 wt.%, as higher water concentrations may shift the reaction equilibrium backward and reduce the overall production yield [3]. In process configurations employing a conventional reactor, this separation is achieved via a distillation column. In contrast, in reactive distillation systems, separation occurs in situ within the column, eliminating the need for a dedicated separation step. Methanol recovery remains an important design target in solvent-intensive processes, and recent studies continue to compare distillation-based and intensified separation routes in terms of energy demand and economic performance [17]. This supports the use of a dedicated methanol-recovery section in the present process design.

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In the second separation stage, the remaining stream primarily composed of methanol and water must be separated to recover methanol for recycle back into the process. For this purpose, two technologies were evaluated: conventional distillation, which relies on differences in boiling points, and pervaporation, which offers higher separation efficiency and lower energy consumption, particularly for near-azeotropic mixtures [18].

Despite the potential advantages of pervaporation, limitations related to membrane commercialization and challenges associated with industrial implementation led to the exclusion of this technology from the final process configuration. Instead, conventional distillation was selected as the preferred option for methanol recovery. Due to the availability of equipment, extensive operational experience, and lower capital and operating costs, this method is considered a reliable choice for industrial applications. The comparison reported by Aeamsuksai et al. [19] demonstrates the quantitative advantages of the reactive distillation configuration over the conventional reactor-based process. Under the optimum operating conditions, the conventional configuration, consisting of an equilibrium reactor followed by two distillation columns, required a CH_3OH/NaOH feed ratio of 4 and exhibited a total energy consumption of 2229.37 GJ/h. In contrast, the reactive distillation configuration, consisting of one reactive distillation column and one conventional distillation column, achieved the same $NaOCH_3$ production rate (675 kg/h) with a substantially lower CH_3OH/NaOH feed ratio of 1.4 and a total energy consumption of only 35.13 GJ/h. This significant reduction in energy demand is attributed to the simultaneous reaction and separation occurring within the reactive distillation column, which significantly decreases the amount of unreacted methanol requiring recycle. Furthermore, Aeamsuksai et al. [19] reported that the third and fourth process configurations were not technically satisfactory because they failed to reduce the water content of the sodium methoxide–methanol solution to the required specification, despite higher methanol consumption.

For methanol–water separation, both distillation and pervaporation membrane technologies were considered. However, although pervaporation has demonstrated promising performance for methanol/water separation, its limited industrial commercialization and scale-up challenges were considered important limitations for large-scale application. Therefore, the distillation-based separation route was selected due to its higher industrial maturity and established operation at commercial scale. Accordingly, the final process configuration adopted in this study consists of a reactive distillation column for sodium methoxide formation, followed by a conventional distillation column for methanol recovery. This configuration was selected as the most technically feasible option considering process performance, product quality requirements, and industrial applicability.

Drying is one of the critical unit operations in chemical and pharmaceutical industries, aimed at removing moisture from solutions or solid materials to improve storage stability, handling, and end-use performance. The selection of an appropriate dryer depends on the physical and chemical properties of the feed, permissible process temperatures, and production capacity [20].

Spray drying was considered a suitable option for the solidification of sodium methoxide. This drying method enables the direct conversion of high-moisture solutions or suspensions into powder or granular products in a single step and offers relatively simple process control and operation [21]. In spray drying, the liquid feed is atomized into fine droplets, and moisture is evaporated upon contact with a hot gas stream. This technique allows the production of uniform particles with narrow size distribution, high purity, and low residual moisture, while eliminating the need for auxiliary operations such as milling or sieving. Furthermore, key product characteristics including particle size, porosity, and residual moisture can be controlled by adjusting operating conditions. Spray dryers are also well

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suited for scale-up and continuous operation, making them an appropriate choice for the industrial production of solid sodium methoxide [22]. Recent studies have also highlighted the importance of process safety in spray drying operations involving flammable solvents or reactive materials. Such systems require careful control of ignition hazards, typically through closed-loop operation with inert gas. Nitrogen blanketing and oxygen concentration control have been identified as key strategies for ensuring the safe industrial operation of spray dryers handling flammable solvent-based feeds [23].

In spray drying processes, the drying gas comes into direct contact with the product, resulting in the evaporation of methanol solvent along with moisture. The release of these flammable vapors into the environment poses safety risks and leads to the loss of valuable materials, thereby reducing overall process efficiency. Therefore, as illustrated in Fig. 2, the design of a closed-loop spray drying system is recommended as a safe and efficient solution [24].

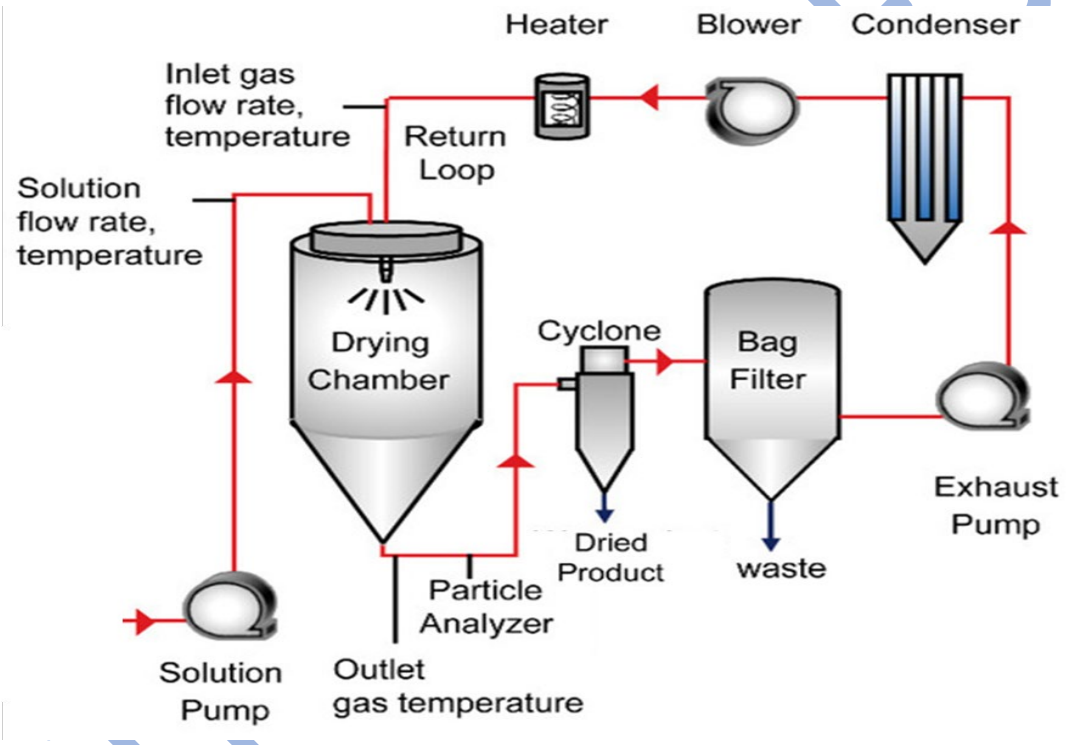


Fig. 2. Schematic diagram of the closed-loop spray drying process [24].

Since sodium methoxide can react with CO_2 and poses an explosion risk due to the presence of methanol and oxygen in air, nitrogen is considered the most suitable drying gas for the sodium methoxide drying process [25]. In addition, sodium methoxide decomposes at temperatures above 350 °C [26]. Therefore, the temperature of the drying gas must be maintained below this threshold.

Although sodium methoxide is commercially available mainly as a liquid methanol solution, the increasing demand for solid sodium methoxide in applications such as pharmaceutical industries and chemical synthesis highlights the need for developing efficient production strategies for this product form. Previous studies have mainly focused on the production of liquid sodium methoxide solutions, while limited attention has been given to the design and techno-economic assessment of integrated processes capable of producing solid sodium methoxide. In addition, the economic impact of providing different product forms according to market requirements has not been sufficiently investigated.

Therefore, the main objective of this study is to design and evaluate an integrated industrial process for the production of solid sodium methoxide from methanol and sodium hydroxide solution. The proposed process integrates reactive distillation for sodium methoxide formation with a spray drying unit for solid product generation. Furthermore, the flexibility of the proposed process to produce either liquid methanol sodium methoxide or solid sodium methoxide based on market demand is investigated. A comprehensive techno-economic analysis is performed to evaluate the economic feasibility of the proposed production scenarios and to determine the effect of product flexibility on the overall process performance.

2. Methodology

Simulation, as an effective tool for the analysis and design of industrial processes, enables detailed investigation of mass and heat transfer phenomena, prediction of system performance, and reduction of the need for costly experimental trials. The objective of the simulation in this study is to model the sodium methoxide production process and to technically evaluate system behavior under various operating conditions prior to conducting the economic assessment.

In this research, a chemical plant utilizing methanol and aqueous sodium hydroxide as feedstocks for sodium methoxide production is investigated. The overall process structure consists of unit operations for the synthesis of sodium methoxide solution, stream separation, and product solidification. Accordingly, the sodium methoxide production process is examined and evaluated in two main sections: the production of sodium methoxide solution followed by its solidification unit.

As discussed in the section 1.2, Configuration 1 (Table 1), consisting of reactive distillation, distillation, and drying units, was initially considered based on the process scheme reported by Granjo et al. [3] . This configuration was selected for further investigation due to its capability to effectively remove water and achieve the required solid sodium methoxide specification (<0.1 wt.% water content). Moreover, previous studies have demonstrated that the reactive distillation configuration can provide advantages over conventional reactor-based processes in terms of lower energy demand and reduced methanol consumption. Therefore, the proposed configuration was developed and evaluated using ASPEN Plus simulation. In this framework, operating parameters such as temperature, pressure, stream flow rates, and initial feed moisture content were adjusted for each unit to ensure optimal production conditions, process stability, and final product quality. Specifically, the process was optimized in two respects: (i) the drying-gas flow rate, inlet temperature, and spray-tower geometry of the solidification unit were adjusted via the ASPEN Plus sensitivity-analysis tool to minimize energy consumption subject to meeting the target product water/solvent content; and (ii) the number of theoretical stages, feed-stage location, and reflux ratio of columns D-501/D-502 were adjusted to minimize methanol loss and utility consumption while meeting the 0.1 wt.% water-content specification.

2.1. Modeling of the sodium methoxide solution production unit

The equipment configuration considered for this unit is presented in Fig. 3. Reactive distillation is one of the most advanced technologies for simultaneous synthesis and product separation. The reactive distillation column (denoted as D-501) and the methanol recovery distillation column (denoted as D-502) were simulated using the RadFrac model. RadFrac is a rigorous and flexible model for simulating multistage vapor–liquid or vapor–liquid–liquid

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separation processes, such as extractive distillation, azeotropic distillation, reactive distillation, and absorption columns.

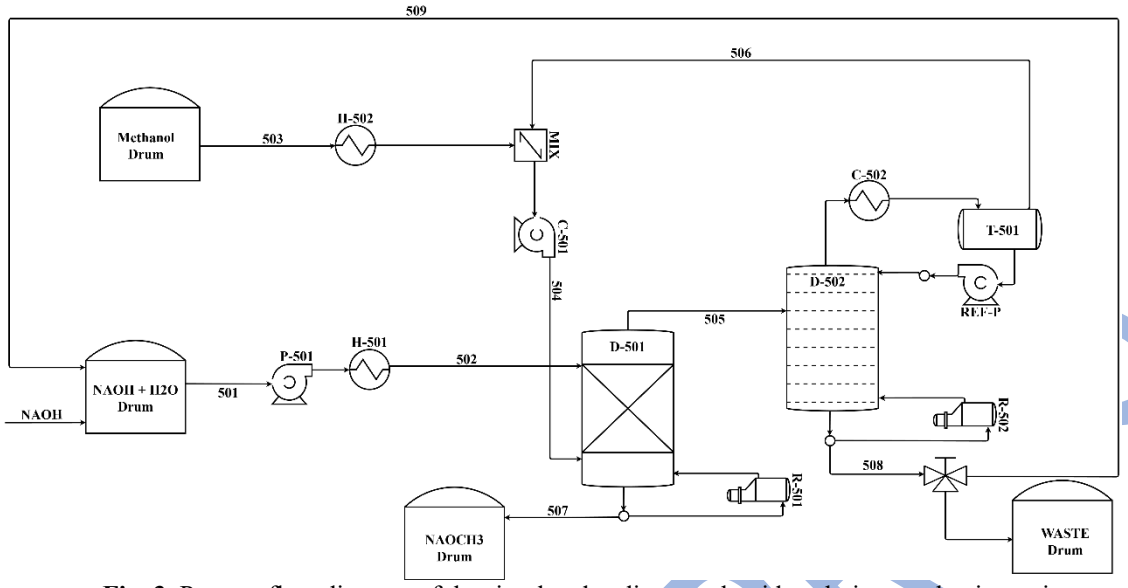


Fig. 3. Process flow diagram of the simulated sodium methoxide solution production unit

Electrolyte reactions in solution (i.e., water self-ionization and salt dissociation) were specified in the Reaction Chemistry section of the ASPEN Plus process simulator. In contrast, the methoxylation reaction was defined as a Reac-Dist type reaction in the Reactions section and incorporated into the RadFrac model of column D-501. The operating pressure of both columns D-501 and D-502 was set to atmospheric pressure (1 bar), as this reaction proceeds rapidly under atmospheric conditions. As shown in the process configuration, column D-501 is operated without a condenser, whereas column D-502 is equipped with a partial condenser. The aqueous sodium hydroxide feed, after being preheated, enters column D-501 from the top, while methanol vapor is introduced from the bottom of the column and is subsequently recovered in column D-502. The unreacted methanol recovered from the separation section is recycled to the process feed (Stream 506), thereby reducing fresh methanol consumption. The main product exits from the bottom of the reactive distillation column D-501 as a sodium methoxide solution in methanol. The water stream separated in column D-502 (From the bottom of column D-502) is divided into two parts. One portion (Stream 509) is recycled and reused for preparing the 50 wt.% sodium hydroxide feed solution, while the remaining excess water (Stream 508) is discharged from the process. This purge stream is required because water is continuously generated during the sodium methoxide synthesis reaction, and complete recycling would result in water accumulation within the process. Accordingly, the purge flowrate was determined from the overall process mass balance rather than through optimization. In addition, a vapor compressor (C-501) and a pump (P-501) were incorporated into the process flow diagram to provide the required pressure for the inlet streams to column D-501.

2.1.1. Reaction chemistry

When sodium hydroxide is added to a methanol–water mixture, an ionic equilibrium is rapidly established between hydroxide and methoxide ions [3]:

$$CH_3OH + H_2O \xrightleftharpoons{K_{hm}} CH_3O^- + H_2O \quad (1)$$

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In addition, both solvents undergo autoprotolysis reactions in methanol–water mixtures, which can be expressed as follows:

$$CH_3OH + H_2O \xrightleftharpoons{K_a} H_3O^+ + CH_3O^- \quad (2)$$

$$2H_2O \xrightleftharpoons{K_w} H_3O^+ + OH^- \quad (3)$$

Since only two of the three reactions represented by Equations (1)-(3) are independent, only Reactions (1) and (3) were implemented in the Aspen Plus simulation. To comply with the electrolyte reaction input format required by Aspen Plus, Reaction (1) was rewritten as:

$$CH_3OH + Na^+ + OH^- \xrightleftharpoons{K_{hm,c}} NaOCH_3 + H_2O \quad (4)$$

The D-501 column was simulated using the RadFrac model, which simultaneously solves vapor–liquid equilibrium (VLE) and chemical reactions on each stage of the column. The electrolyte reaction (Equation (3)), were specified in the Reaction Chemistry input form, allowing the ionic species to be calculated consistently within the eNRTL thermodynamic framework.

In contrast, the main sodium methoxide formation reaction (Equation (4)) was defined in the Reactions input form as a Reac-Dist reaction and assigned to the RadFrac model of column D-501. This implementation enables the reaction to be solved simultaneously with the vapor–liquid equilibrium calculations on each stage of the column, rather than in a separate reactor.

In this study, chemical equilibrium in D-501 was assumed to be instantaneous. Therefore, the extent of reaction on each stage is determined solely by the chemical and phase equilibria. Accordingly, the reaction equilibrium was calculated using the equilibrium constants given by the following correlations:

$$\ln K_{hm,c} = -4.374 + 1751/T \quad (5)$$

$$\ln K_{w,x} = 132.89888 - 13445.9/T - 22.477301 \ln T \quad (6)$$

2.2. Modeling of the solid sodium methoxide production unit

The overall schematic of the product solidification unit is shown in Fig. 4. The system comprises the main units including a heater (H-601), a spray dryer (S-601), a cooler (Cool-601), and a flash tank (F-601). The make-up drying gas stream (601), together with the recycled drying gas stream (603), enters the heater (H-601), where its temperature is raised to the desired level prior to entering the spray dryer. The feed stream (602) is also introduced into the spray dryer.

In the spray dryer, the incoming liquid feed containing the sodium methoxide solution is atomized into fine droplets by a rotary atomizer and comes into direct contact with the hot gas stream. Consequently, the solvent present in the droplets is evaporated, and the dried product (sodium methoxide powder) is collected at the bottom of the drying chamber.

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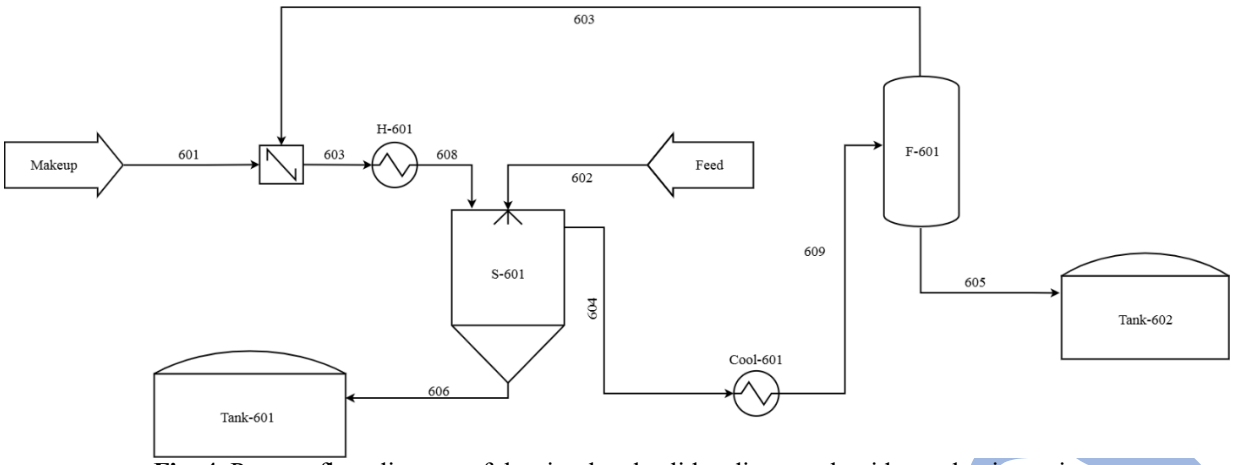


Fig. 4. Process flow diagram of the simulated solid sodium methoxide production unit.

The gas stream leaving the top of the spray dryer, containing methanol vapor and a certain amount of moist gas (604), is directed to the cooler (Cool-601) to reduce its temperature. This temperature reduction leads to the condensation of methanol vapor and facilitates its separation in the subsequent stage. The cooled stream is then transferred to the flash tank (F-601). In this unit, vapor–liquid separation takes place, where the liquid phase, mainly consisting of recovered methanol, is withdrawn from the bottom of the vessel, while the dry gas stream (603) exits from the top and can be recycled back to the drying gas loop.

The developed model enables detailed analysis of key operating parameters, including evaporation efficiency, methanol recovery rate, outlet product temperature, and the quality of the recycled gas stream.

3. Results and Discussion

3.1. Process model validation

To validate the process model developed in ASPEN Plus, the simulation results reported in a previous study [3] were selected as the benchmark for comparison. Their simulation framework had previously been validated against pilot-scale experimental data, providing a reliable reference for assessing the consistency of the present model. The overall process configuration presented in the reference study includes two distillation columns for sodium methoxide production, which is consistent with the process flow diagram proposed in the present work. The model input specifications including mass flow rates of process streams, operating conditions (temperature and pressure), the number of theoretical stages (NT) in columns D-501 and D-502, and the feed stage location (NF), and the reflux ratio of column D-502 were extracted from the reference study and implemented in the current simulation model [3]. The results of the model validation for a 5 $kt.y^{-1}$ production unit are summarized in Table 2, demonstrating good agreement between the simulation outcomes and the reference data. Although the relative error for the NaOH concentration is 29%, the absolute deviation is only 9 ppm (40 vs. 31 ppm). Since NaOH is present only as a trace impurity, the predicted NaOH concentration (31 ppm) remains far below the maximum allowable limit for unreacted alkali (0.4 wt.%). In addition, the residual water content remains below the specified limit (0.1 wt.%) [3]. Therefore, this discrepancy does not affect the assessment of product quality or the conclusions of the study.

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Table 2. Comparison of simulation results for the first configuration between the present study and the data reported by Oliveira and Grangeiro [3].

	Reference result	Simulation result	Abs Eror (%)
D-501			
Distillate temperature (°C)	70.7	73	3.4
Bottoms temperature (°C)	95.5	95.7	02
Distillate mass flow (kg.h-1)	14281	14284	0.021
Product mass flow (kg.h-1)	4010	4010	0.13
Water content in product (ppm)	547 ppm	658	16
NaOH in product (ppm)	40	31	29
NaOCH3 in product (wt%)	0.298	0.303	1.65
D-502			
Distillate temperature (°C)	65	64.6	0.62
Bottoms temperature (°C)	100	99.8	0.2
Distillate mass flow (kg.h-1)	13548	13546	0.015
Bottoms mass flow (kg.h-1)	733	738	0.68
Water content in distillate (ppm)	95	83	14.5
Methanol content in bottoms (ppm)	979	827	18.4

3.2. Simulation results

After validation of the model implemented in ASPEN Plus, the simulation was applied to two production capacities of 10 and 15 kt.y^{-1}. The model input parameters corresponding to these capacities are presented in Table 3.

Table 3. Operating conditions of the equipment used in the sodium methoxide solution production unit at capacities of 10 and 15 kt.y^{-1}.

Equipment	Operating condition	Value	
		10 kt.y^{-1}	**15 kt.y^{-1}**
D-501	Pressure (bar)	1.01	1.01
	NT	20	20
	Condensor	None	None
	Reboiler	Kettle	Kettle
	Distillate rate (kg.h^{-1})	16490	22050
D-502	Pressure (bar)	1.01	1.01
	NT	32	32
	NF	26	26
	Reflux ratio	1.025	1.025
	Distillate rate (kg.h^{-1})	15150	20035
H-501	Temperature output	75	75
	Pressure output	3.04	3.04
H-502	Temperature output	65	65
	Pressure output	1.01	1.01
P-501	Pressure increase (bar)	2.03	2.03
C-501	Pressure increase (bar)	2.03	2.03
	Type	Isentropic	Isentropic

The simulation results for each production capacity are presented in Tables 4 and 5, respectively. As shown in these tables, the sodium methoxide production flow rate is 1234.4 kg.h-1, which assuming 8,000 operating hours per year for the industrial unit corresponds to an annual production of approximately 10 kt of sodium methoxide. Moreover, the mass fraction of water in the final product stream is below the specified allowable limit, indicating that the quality of the produced product falls within an acceptable range.

Table 4. simulation results of the sodium methoxide solution production unit with a capacity of 10 kt.y^{-1}.

Stream	**501**	**503**	**504**	**505**	**506**	**507**	**508**	**509**
Temperature (C)	30	30	158.6	74.6	64.6	97.2	99.9	99.9
Pressure (bar)	1.01	1.01	3.04	1.01	1.01	1.01	1.01	1.01
Vapor fraction	0	0	1	1	1	1	0	0
Mass flow (kg.h^{-1})	1850	3500	18650	16490	15150	4010	1340	925
Component Mass Flow (kg.h^{-1})								
H2O	925	0	7.25	1347	7.25	1.6	1340	925
NaOH	925	0	0	0	0	15.5	0	0
NaOCH3	0	0	0	0	0	1234.4	0	0

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CH3OH	0	3500	18642	15143	15142	2759	6e-3	6e-3
Mass fraction								
H2O	0.5	0	5e-4	0.08	4e-4	4e-4	0.999	0.999
NaOH	0.5	0	0	0	0	0.004	0	0
NaOCH3	0	0	0	0	0	0.308	0	0
CH3OH	0	1	1	0.92	1	0.688	4e-6	4e-6

Table 5. simulation results of the sodium methoxide solution production unit with a capacity of 15 kt.y^{-1}.

Stream	**501**	**503**	**504**	**505**	**506**	**507**	**508**	**509**
Temperature (C)	30	30	158.6	75.1	64.6	97.2	99.7	99.7
Pressure (bar)	1.01	1.01	3.04	1.01	1.01	1.01	1.01	1.01
Vapor fraction	0	0	1	1	1	0	0	0
Mass flow (kg.h^{-1})	2775	5250	18650	22050	20035	6010	2015	1391
Component Mass Flow (kg.h^{-1})								
H2O	1387.5	0	7.25	2014	2.9	0.87	2011	1387.5
NaOH	1387.5	0	0	0	0	10.5	0	0
NaOCH3	0	0	0	0	0	1864	0	0
CH3OH	0	5250	18642	20035	20032	4135	3.4	3.5
Mass fraction								
H2O	0.5	0	5e-4	0.09	1.5e-4	4e-4	0.998	0.998
NaOH	0.5	0	0	0	0	0.0016	0	0
NaOCH3	0	0	0	0	0	0.31	0	0
CH3OH	0	1	1	0.91	1	0.688	1.6e-3	1.6e-3

Following the simulation of the liquid sodium methoxide production unit, the solidification unit was simulated. The feed to this unit is liquid sodium methoxide, which corresponds to the product stream of the previous unit. It should be noted that this unit was simulated for a solid sodium methoxide production capacity of 10 kt.y^{-1}. The model input data are reported in Table 6.

The values assigned to the model parameters of each equipment item were determined using the sensitivity analysis tool of ASPEN Plus, with the objective of minimizing unit energy consumption while achieving the desired product quality.

Table 6. Operating conditions of the equipment used in the solid sodium methoxide production unit.

Equipment	**Operating condition**	**Value**
S-601	Pressure (bar)	1
	Spray tower height (m)	5
	Spray tower diameter (m)	2
	Ambient temperature (°C)	55
	Heat transfer coefficient (cal/sec.sqcm.k)	16490
	Atomizer type	Rotary
	Number of atomizers	1
	Atomizer wheel diameter (m)	0.5
	Number of blades	5
	Blade height (m)	0.03
	Wheel speed (rpm)	4000
H-601	Temperature output (°C)	260
	Pressure output (bar)	1
Cool-601	Temperature output	-15
	Pressure output (bar)	1
F-601	Pressure (bar)	1
	Duty (Kw)	0

The numerical results obtained from the simulation are presented in Table 7. According to these results, the mass flow rate of the gas entering the spray dryer is 17,000 kg.h^{-1}, resulting in a gas-to-feed mass ratio of 4.2, where the feed stream contains the sodium methoxide solution. In this process, nitrogen was selected as the drying gas, and its inlet temperature to the spray dryer was set at 260 °C, while the outlet gas temperature from the spray dryer was 82.2 °C (stream 604). This temperature was chosen to provide sufficient energy for methanol evaporation while preventing the thermal degradation of sodium methoxide. The solid sodium methoxide product obtained from the

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spray dryer has a simulated composition of 99.8 wt.% $NaOCH_3$ with 0.2 wt.% residual methanol (Table 7, stream 606), indicating a high-purity product. This simulated purity exceeds the typical commercial specification for solid sodium methoxide (≥97 wt.% assay). The methanol evaporated from the sodium methoxide solution was carried with the nitrogen in the spray dryer exhaust gas (stream 604). The exhaust gas was subsequently cooled and fed to a flash tank, where condensed methanol was separated from the nitrogen stream. The recovered methanol (stream 605) was sent to a storage tank, while the nitrogen was recycled to the spray dryer in the closed-loop system. Based on the recovered methanol stream, the methanol recovery was approximately 99.9%. In the dryer model, steady-state operation, negligible heat loss, complete methanol evaporation from droplets, and complete recovery of solid particles were assumed.

Table 7. Complete simulation results of the solid sodium methoxide production unit

Stream	601	602	603	604	605	606	607	608
Temperature (C)	9	70	-14.7	82.2	-15.08	82.2	69	260
Pressure (bar)	1	1	1	1	1	1	1	1
Vapor fraction	1	0	1	1	0	0	1	1
Mass flow (kg.h-1)	4.5	4010	16993	19756	2760	1254	16997	16997
Component Mass Flow ($kg.h^{-1}$)								
N2	4.5	0	16747	16753	4	0	16751	16751
NaOCH3 (L)	0	1251	0	0	0	0	0	0
NaOCH3 (S)	0	0	0	0	0	1251	0	0
CH3OH	0	2759	246.6	3002.6	2756	2.6	246	246
Mass fraction								
N2	1	0	0.9855	0.848	0.0016	0	0.9855	0.9855
NaOCH3 (L)	0	0.312	0	0	0	0	0	0
NaOCH3 (S)	0	0	0	0	0	0.998	0	0
CH3OH	0	0.688	0.0145	0.152	0.9984	0.002	0.0145	0.0145

3.3. Economic evaluation

Following the technical assessment of the models developed for each process unit, the next step is to evaluate the process from an economic perspective. In this study, capital investment costs and operating costs were estimated using ASPEN Plus software. The prices of the consumed raw materials and the produced product are presented in Table 8.

Table 8. Raw material costs and product price

Chemical	Cost ($ t−1)
Sodium hydroxide (50 wt%)	378
Methanol	260
Sodium metoxide (30 wt%)	900
Sodium metoxide	3300
Price in $Nm−3 calculated from eNm−3 [36].	

The economic evaluation was performed based on conceptual design assumptions, including 100% production capacity after commissioning, an annual operating time of 8000 h/year, the assumed product selling prices and raw material costs, and a short EPC implementation period of 21 weeks. In addition, working capital was considered as part of the total capital investment. According to the Aspen Process Economic Analyzer (APEA) assumptions, the required working capital was estimated as 5% of the capital cost, and this value was included in the payback period calculation. Therefore, the calculated IRR and payback period should be interpreted as indicators of the economic potential of the proposed process under the adopted assumptions rather than as definitive investment decisions. The economic analysis was performed considering the defined system boundaries of the proposed production process.

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The operating cost includes the consumption of raw materials, utilities, labor, maintenance, and other process-related operating expenses estimated using APEA. The analysis also accounts for methanol recovery through the recycle system, which reduces fresh methanol consumption. Costs associated with product packaging, transportation, distribution, and other downstream commercial activities were not included, as they depend on the specific implementation scenario and are outside the scope of the present study.

3.3.1. Economic evaluation of the sodium methoxide solution production unit

In estimating the capital investment costs of the sodium methoxide solution production unit, major equipment items including the vapor compressor (C-501), pump (P-501), heat exchangers (H-501 and H-502), distillation columns (D-501 and D-502) along with their associated reboilers (REB-501 and REB-502), condenser (COND-502), and the reflux drum (DRUM-502) related to column D-502 were considered. The dimensions of these equipment items were determined using the ICARUS process evaluation system embedded in ASPEN Plus.

The reactive distillation column D-501 was selected as a structured packed column, as it operates at low liquid flow rates, offers high hydraulic capacity, and provides favorable vapor flow characteristics. These features help prevent excessive residence time distribution within the column. Column D-502 was considered as a sieve tray column, since this type of column has lower capital and maintenance costs and is well suited for handling high liquid flow rates.

All equipment used in this process was assumed to be constructed of stainless steel, because solutions containing sodium hydroxide and methanol can cause corrosion in carbon steel. However, the shells of the heat exchangers were made of carbon steel, as the low-pressure steam used in H-501, H-502, REB-501, and REB-502, as well as the cooling water employed in COND-501, are not corrosive to this material [3]. Table 9 presents the costs of the equipment employed in this unit along with their installation costs.

Table 9. Equipment capital investment costs for the sodium methoxide solution production unit at production capacities of 10 and 15 kt.y^{-1}.

Equipment	Equipment Cost ($K)		Installed Cost ($K)	
	10 kt.y^{-1}	15 kt.y^{-1}	10 kt.y^{-1}	15 kt.y^{-1}
C-501	2211	2698.7	2516	3029.1
P-501	5.3	5.3	36.8	36.8
REB-501	25	33.6	124	137.1
REB-502	36	41.2	153	162.1
COND-502	57	70.8	172	216.3
H-501	10.5	11.2	62.3	63.1
H-502	15.2	17.6	87.2	103.4
D-501	552	708.3	888	1090.1
D-502	466	554.2	878	1007.6
DRUM-502	20.5	21.1	144	144.8
REF-P	8	8.5	53	55.3
Total	3407	4170.5	5115	6045.7

Table 10 presents the utility consumption and the associated costs for two production capacities of 10 and 15 kt.y^{-1}. As can be observed, increasing the production capacity from 10 to 15 kt.y^{-1} leads to an increase in the total utility cost from USD 2.361 million per year to USD 3.164 million per year. However, the increase in utility costs is lower than the corresponding increase in production capacity. These results confirm that scaling up the production capacity, despite the absolute increase in energy consumption, remains economically justifiable from the perspective of utility operating costs.

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Table 10. Utility consumption costs for the sodium methoxide solution production unit at production capacities of 10 and 15 kt.y^{-1}.

Utility	Rate		Cost per Hour	
	10 kt.y^{-1}	15 kt.y^{-1}	10 kt.y^{-1}	15 kt.y^{-1}
Electricity (KW)	938	1126	72.69	87
Cooling Water (MMGAL/h)	0.097034	0.13	11.6441	15.4
Steam (KLB/h)	25.928	36	210.885	293.2
Total ($K/year)			2361	3164

Table 11 summarizes the capital investment and operating costs of the sodium methoxide production unit for two production capacities of 10 and 15 kt.y^{-1}. As observed, increasing the production capacity results in an increase in all cost components, including total capital investment, operating costs, and utility costs. Overall, the comparison between the two capacities indicates that although capacity expansion leads to higher absolute costs, the rate of cost increase is lower than the corresponding increase in production capacity. This trend reflects an improvement in economic performance indicators and highlights the greater attractiveness of the higher capacity for industrial investment.

Table 11. Capital and operating costs of the sodium methoxide solution production unit at production capacities of 10 and 15 kt.y^{-1}.

Investment	Cost ($K)	
	10 kt.y^{-1}	15 kt.y^{-1}
Total Capital Cost ($)	16000	17900
Total Operating Cost ($/Year)	5476	7037
Utility Cost ($/Year)	2361	3164
Equipment Cost ($)	3407	4170
Total Installed Cost ($)	5115	6045

3.3.2. Economic evaluation of the drying unit with a capacity of 10 kt.y^{-1}

In estimating the capital investment costs of the solidification unit for liquid sodium methoxide, major equipment items including heat exchangers (H-601 and Cool-601), the spray dryer (S-601), and the flash vessel (F-601) were considered. All equipment used in this process was assumed to be constructed of stainless steel, as solutions containing sodium methoxide and methanol can cause corrosion in carbon steel. However, the shells of the heat exchangers were made of carbon steel, since the low-pressure steam used in H-601 and the cooling water employed in Cool-601 are not corrosive to this material.

Table 12 presents the capital investment costs of the equipment used in this unit. Among the equipment items, the spray dryer (S-601) accounts for the largest share of the total cost, representing the major portion of the initial capital investment.

Table 12. Equipment capital investment costs for the solidification unit at a production capacity of 10 kt.y^{-1}.

Equipment	Equipment Cost ($K)	Installed Cost ($K)
S-601	2130	2592.2
F-601	34.2	207.4
H-601	36.1	160
C-601	23.5	109.3
Total	2223.8	3068.9

Table 13 presents the process utility costs, including electricity and the refrigerant Freon-12. Based on the data, the annual operating cost is estimated at approximately USD 89.4 thousand, a significant portion of which is attributed to

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cooling energy consumption (refrigerant usage). These costs are incorporated into the calculation of the annual operating expenses and play an important role in determining the final product cost.

Table 13. Utility consumption costs for the solidification unit at a production capacity of 10 kt.y^{-1}.

Utility	Rate	Rate Units	Cost per Hour	Cost Units
Electricity	52.3	kW	4.05	$/h
Refrigerant-Freon12	32.79	Kg.h^{-1}	6.15	$/h
Total ($K/year)	89.4			

Table 14 presents the overall estimation of capital investment and operating costs for a production capacity of 10 kt.y^{-1}. The total capital investment is estimated at USD 8.72 million, while the annual operating costs amount to USD 3.892 million.

Table 14. Capital and operating costs of the solidification unit at a production capacity of 10 kt.y^{-1}.

Investment	Cost ($K)
Total Capital Cost ($)	8720
Total Operating Cost ($/Year)	3892
Utility Cost ($/Year)	89.4
Equipment Cost ($)	2224
Total Installed Cost ($)	3069

After conducting separate techno-economic assessments of each sodium methoxide production unit, a final integrated assessment of the entire process was performed for a total production capacity of 15 kt.y^{-1}. Of this capacity, 10 kt were allocated to solid sodium methoxide production and 5 kt to liquid sodium methoxide production.

3.3.3. Overall economic evaluation of the entire process

In this section, a comprehensive economic evaluation of the project over a 20-year operating period is presented. Key financial indicators, including the IRR and the payback period (PBP), were calculated to assess the profitability and investment attractiveness of the project. The IRR reflects the project's ability to generate returns exceeding the cost of capital and is regarded as a primary criterion for evaluating financial feasibility. The PBP represents the time required for the initial investment to be recovered through net cash flows.

As shown in Table 15, the total capital investment of the entire project is estimated at USD 26.62 million, while the annual operating costs amount to approximately USD 32.195 million. Raw material costs constitute the largest portion of the operating expenses, accounting for USD 21.266 million per year. In contrast, annual product sales, valued at USD 58.710 million, provide a substantial profit margin for the project, highlighting the strong economic attractiveness of the proposed process.

Table 15. Total capital and operating costs of the integrated process for producing 5 kt.y^{-1} of liquid and 10 kt.y^{-1} of solid sodium methoxide.

Investment	Cost ($K)
Total Capital Cost ($)	26620
Total Operating Cost ($/Year)	32195
Total Raw Materials Cost ($/Year)	21266
Total Product Sales ($/Year)	58710
Utility Cost ($/Year)	3253
Equipment Cost ($)	6394
Total Installed Cost ($)	9114
PBP (Year)	1.58
IRR (%)	175

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In the base-case economic analysis, the plant was assumed to operate under continuous operation conditions at full capacity (100% capacity factor). To investigate the effect of operational availability on the project economics, the payback period was recalculated at 85% capacity utilization.

The reduction in production capacity decreases annual production and revenue, resulting in a longer payback period and a lower internal rate of return compared with the base case. The sensitivity analysis showed that at 85% capacity utilization, the payback period increased to 2.05 years, while the internal rate of return decreased to 127%. These results indicate that the proposed process still maintains favorable economic performance even under reduced plant utilization conditions.

4. Conclusions

The results indicate that the project payback period is approximately 1.58 years, demonstrating a rapid recovery of the initial investment. In addition, the IRR was calculated to be 175%, which is significantly higher than the typical return rates in the chemical industry. These results suggest that the proposed process has strong techno-economic potential for industrial implementation. Nevertheless, the economic performance remains dependent on the assumptions adopted in this study, including product selling prices, raw material costs, plant operating capacity, and capital cost estimation. Therefore, the reported economic indicators should be interpreted as reflecting the techno-economic potential of the proposed process under the assumed design basis rather than as definitive investment metrics. Further sensitivity and uncertainty analyses, together with pilot-scale validation, are recommended to confirm the robustness of the findings under practical industrial conditions. This study has several limitations: the ASPEN Plus model was verified against previously published simulation results rather than experimental or plant data; the original economic evaluation did not include a systematic sensitivity or uncertainty analysis; and environmental life-cycle and formal process-safety (HAZOP) assessments were outside its scope. Future work should include experimental or pilot-scale validation, evaluation of capacity expansion and product diversification, a comparative life-cycle assessment of alternative production routes, and a formal process hazard analysis. While the base-case economic indicators are based on the assumptions adopted in this study, the sensitivity analyses presented in the Supporting Information demonstrate that the project remains economically attractive over a reasonable range of the key economic and operating parameters, confirming the robustness of the findings.

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Nomenclature

Symbols		Abbreviation	
T	Temperature (K)	ASPEN Plus	Process simulation software
K_{hm}	Equilibrium constant of the methanol–hydroxide/methoxide ionic-equilibrium reaction (Eq. 1)	APEA	Aspen Process Economic Analyzer
K_a	Equilibrium constant of the methanol–water autoprotolysis reaction (Eq. 2)	CAGR	Compound Annual Growth Rate
K_w	Equilibrium constant of the water self-ionization reaction (Eq. 3)	eNRTL	Electrolyte Non-Random Two-Liquid

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$K_{hm,c}$	Concentration-based equilibrium constant of the methoxylation reaction, electrolyte-reaction form (Eq. 4)	EPC	Engineering, Procurement, and Construction
$K_{w,x}$	Mole-fraction-based equilibrium constant of the water self-ionization reaction	HAZOP	Hazard and Operability
C	Compressor	IRR	Internal Rate of Return
P	Feed pump	NF	Feed-stage location
H	Heater	NT	Number of theoretical stages
D	Distillation column	PBP	Payback Period
S	Spray dryer	RadFrac	Rigorous multistage vapor–liquid(–liquid) equilibrium distillation model in ASPEN Plus
REB	Reboilers	TEA	Techno-Economic Assessment
COND	Condenser	VLE	Vapor–Liquid Equilibrium
Cool	Cooler		
F	Flash tank		

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