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Techno-economic analysis of methanol and ammonia co-producing process using CO_2 from blast furnace gas

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Abstract−In steel manufacturing plants, blast furnace gas is generated from a furnace in which steel ore, coke and limestone are heated and melted. It is commonly used to produce electricity or released to the atmosphere in general; however, it can be utilized as a carbon source to produce C1 value-added chemicals. In this study, we propose two production schemes for methanol production and co-production of methanol and ammonia from blast furnace gas. Both cases were simulated using Aspen Plus V12 and economics was evaluated using Aspen Process Economic Analyzer (APEA). As a result, the methanol production case produced 99.4 wt% 232 t/day of methanol and the co-production case produced 97.7 wt%, 453.4 t/day of ammonia and 99.8 wt%, 263 t/day of methanol. The total annual cost of the methanol production case is US 121.6 M$/y and US 222.1 M$/y at the co-production case. The NPVs are −810.4 M$ in the methanol production case and −981.3 M$ in the co-production case, respectively. By sensitivity analysis, it is shown that the co-production case can be more economically feasible in the aspect of NPV when the raw material cost decreases 30%.

Keywords: Ammonia Synthesis, Methanol Synthesis, CO_2 Utilization, Process Simulation, Techno-economic Analysis, Sensitivity Analysis

INTRODUCTION

Global energy consumption grew by 2.3% in 2018, nearly twice the average rate of growth since 2010, driven by a robust global economy as well as higher heating and cooling requirements. As a result of the higher energy consumption, global energy-related CO_2 emissions increased to 33.1 Gt CO_2, up 1.7% from 2017 [1]. Especially, steel manufacturing accounted for over a quarter of the industry's CO_2 emissions [2]. The International Energy Agency's (IEA) 2 °C scenario for 2050 suggests the steel industry to reduce over a third of the CO_2 emissions in the industrial sector (excluding power generation) [2]. In detail, the world steel industry accounts for 5% of the world's total energy consumption and more than 6% of the total CO_2 emissions per year [3]. Moreover, in 2018, steel produced over 1.7 billion tons and its production will grow in the next future [4]. Accordingly, CO_2 emissions to atmosphere and energy consumption will also increase.

As a solution, carbon capture, utilization and storage (CCUS) technology is proposed to avoid more serious climate change and reduce CO_2 emissions [5]. This technology can promote sustainability and the circular economy, encourage industrial symbiosis and economic growth, and enable the storage of renewable energy [6]. Especially, CCU is the technology using CO_2 as a raw material to produce value-added products such as methanol, formic acid, ethanol and dimethyl ether [7]. Several facilities such as Geroges Olah Methanol plant in Iceland, Dream production of polyols and concrete plants for Carboncure's production of mineral carbonates have started to operate with purified and compressed CO_2 [8]. Although CO_2 can convert to value-added chemicals and fuels, the conversion of CO_2 is energy intensive and requires high-selectivity catalysts due to the thermodynamically high stability of CO_2. Moreover, chemicals and fuels have short lifespan, thus it causes limited storage periods for captured CO_2 [9].

In the steel manufacturing process, off-gases such as coke oven gas (COG), basic oxygen furnace gas (BOFG) and blast furnace gas (BFG) are emitted and have different compositions and flow rates [10]. COG is produced in the coke-making process when volatile coal matter is converted into COG, leaving carbon intensive coke behind [11]. Although COG has high H_2 content, it has low concentration of carbon so that it cannot be a suitable carbon source. BOFG is produced in the basic oxygen furnace at which the molten iron from the blast furnace is introduced [12]. BFG is the byproduct gas in the blast furnace in which the crushed iron oxide ore is reduced by coke in the presence of hot air under a liquid limestone bed [13]. It emits ten times more than the sum of the COG and BOFG. So, we developed the CCU process by using the BFG off-gas as a carbon source because BFG has a large amount compared to other off-gases.

This work presents the development of a commercial scale of CCU process combining the methanol production and ammonia production processes using BFG off-gas from a steel manufacturing plant. Methanol is a light, colorless and volatile liquid alcohol with a distinctive scent. It is the simplest type of alcohol and consists of a methyl group combined with a hydroxy group.

It can utilize the production of dimethyl ether (DME) and methyl tert-butyl ether, which are the alternatives of conventional fuel, gaso-

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line [14]. Reference [15] describes the increasing demand of the methanol from 2016 to 2018. Also, methanol demand continuously increases for the near future. There are many studies simulating the methanol process from CO_2.

Lee et al. proposed a techno-economic analysis of the methanol synthesis via CO_2 hydrogenation [16]. They assumed that CO_2 was captured from power plant or air and H_2 was produced from water electrolysis, which electricity was made from renewable energy. To determine the techno-economic feasibility, they simulated the process using ASPEN HYSYS and found the unit production cost, which is the total annual cost divided by total methanol production [16]. The difference with our work is that Lee used direct CO_2 from power plant or air, but we used the syngas from a steel manufacturing plant.

Similarly, Perez Fortes et al. described the techno-economic analysis of methanol synthesis via CO_2 hydrogenation [17]. They compared two methanol production processes with and without the heat integration using CHEMCAD. To determine the economic feasibility, they found the net present value (NPV) and break-even values which the NPV equals zero while changing the economic parameters such as CO_2 price, H_2 price and methanol price [17]. The difference with our work is that Fortes describes the direct CO_2 hydrogenation similar to Lee's paper, while Fortes describes the H_2 is provided by a hypothetical network. It means, they do not consider the H_2 source.

Shin et al. presented a techno-economic analysis of a process using COG and BOFG as carbon sources and producing H_2 by steam methane reforming (SMR) using ASPEN Plus. They calculated the minimum selling price (MSP) of the methanol and estimated it from US 371 $/t to US 398 $/t [18].

Kim et al. presented a techno-economic analysis of a process using BFG as a carbon source and producing H_2 from SMR [21]. They calculated the MSP of the methanol and estimated it from US 902 $/t to US 1,249 $/t. Besides these, there have been works about CCU process and techno-economic analysis of methanol synthesis using various carbon sources [19-21].

Ammonia is the second most common chemical produced in the world, at an estimated global production of 140 million tons in 2018 [22]. Also, the global ammonia market size is expected to reach US 76.64 billion by 2025, at a registering a compound annual growth rate (CAGR) of 5.3% over the future, according to Grand View Research, Inc [23]. With this importance, ammonia producing processes have been studied for decades [24-26].

In this study, we propose a process which produces both methanol and ammonia using BFG from a steel manufacturing plant and present a techno-economic analysis. This process can produce ammonia without additional air separation units and mitigate the CO_2 emission due to the use of CO_2 as a raw material.

For a comparison, two cases are studied: one, the base case produces only methanol based on the study by Kim et al. [21], and the other is the case which adds ammonia synthesis process which is based on [27]. After simulating both cases, heat integration is applied to minimize the energy requirement and NPVs are calculated. Finally, we performed sensitivity analysis of main cost factors that are affected NPV.

The rest of this paper involves the following content. First, the assumption of the process and simulation of methanol production and coproduction of methanol and ammonia are presented in Section 2. Then, the simulation results are discussed in the aspect of techno-economic analysis and sensitivity analysis in Section 3. Finally, concluding remarks are presented in Section 4.

Table 1. Composition and heating value of steel industry off-gases

Component	COG [10]	BOFG [10]	BFG [10]
Composition (vol%)			
H_2	62	1.2	3
CO_2	1.5	16	24
CO	7	67	20
CH_4	26	-	-
N_2	2.2	15	53
O_2	-	0.2	-
H_2O	-	0.6	-
C_2H_6	0.5	-	-
C_2H_4	0.8	-	-
Lower heating value (LHV) (kJ/mol)	397.5	192.7	70.1

METHODS

1. Process Descriptions of Methanol Production

Table 1 shows the composition and heating values of general off-gases. Conventionally, a plant producing 6 Mt/y of steel emits COG, BOFG and BFG at 40,000, 35,000 and 730,000 Nm^3/h, respectively [12]. We assumed all the composition of the off gases that produced in the steelmaking plant are desulfurized. Due to the large amounts of BFG, we used BFG as a carbon source.

First, a base case which only produces methanol from BFG is simulated based on the previous works [20,21]. Then the proposed process which adds ammonia synthesis from BFG is simulated. All of cases were developed based on material and energy balances using a commercial process simulator, ASPEN Plus V12.0 (Aspen Technology, Inc., Bedford, MA, USA) [30].

1-1. Process Simulation of the Base Case

Fig. 1 shows the process flow diagram (PFD) of methanol synthesis from the BFG. As a thermodynamic property model, Non-Random-Two-Liquid (NRTL) model was used for the whole processes, including the reactor, separator, mixer, splitter, compressor and distillation columns [21].

The H_2 (Stream 1 in Fig. 1) generated from the water electrolysis and BFG (Stream 2 in Fig. 1) are mixed in mixer 1 and passed through the four-stage multi-compressor with intercooling. The R parameter is a relation representing the proportions of H_2, CO_2, and CO in the feed in methanol reactor, which is defined as follows $R=(F_{H_2}-F_{CO_2})/(F_{CO}+F_{CO_2})$, where F_i is the molar flow of the component i. Bermudez et al. reported that the by-products are produced when the R parameter is lower than 2 and excessive H_2 is used when it is higher than 2 [20]. Thus, the R parameter of the feed of methanol reactor is fit to 2 by adjusting the molar flow rate of H_2. By four stage multi-compressor unit, the BFG-H_2 mixed stream is compressed and cooled to 100 bar and 520 K, which are equal to a

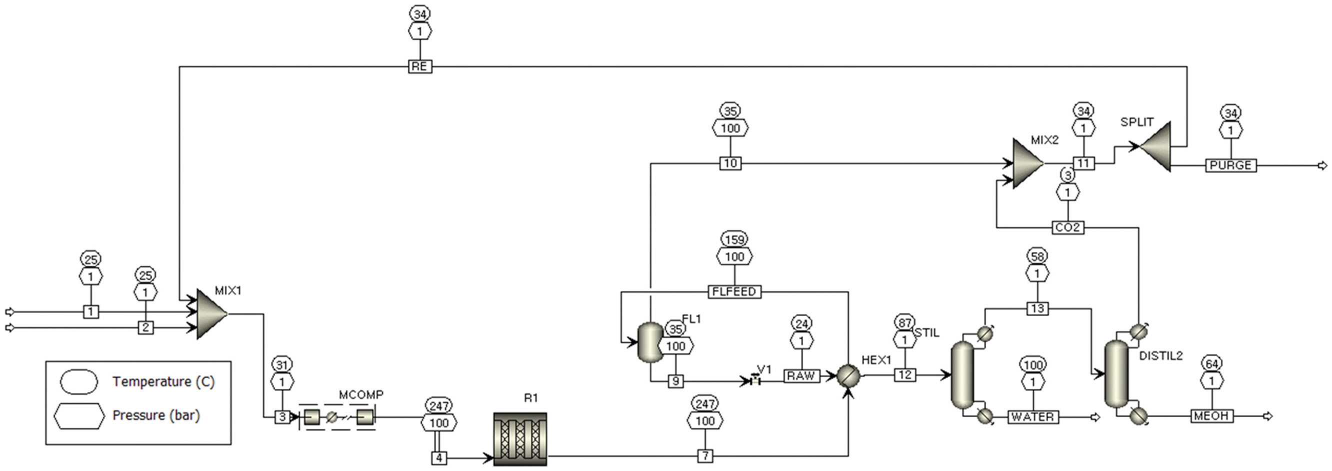

Fig. 1. The PFD of the methanol production case (base).

Table 2. Kinetic factors of Eqs. (4) to (6)

Reaction	k	n	E_a [kJ/mol K]
1	4.0638×10^{-6} [kmol/kg_{cat} s Pa]	0	11.695
2	9.0421×10^{8} [kmol/kg_{cat} s $Pa^{1/2}$]	0	112.86
3	1.5188×10^{-33} [kmol/kg_{cat} s Pa]	0	266.01

methanol reactor's (R1 in Fig. 1) operation conditions that is optimized in the previous study in [21]. The methanol reactor is assumed a multi-tube Lurgi reactor that converts syngas to methanol, and is operated at 503 K$\leq T_{op}\leq$538 K and pressure 50 bar$\leq P_{op}\leq$ 100 bar. This reactor is used in a commercial middle size methanol plant [29,30]. The methanol synthesis reactions occur using a commercial $Cu/ZnO/Al_2O_3$ catalyst, and the kinetics are based on Graaf's kinetic model of methanol synthesis, which are described as follows in Eqs. (1) to (6) [31]. The nominal values parameters are given in Tables 2-4.

$$CO+2H_2 \leftrightarrows CH_3OH \qquad \Delta H_{298\,K}=-90.77\ \text{kJ/mol} \tag{1}$$

$$CO_2+H_2 \leftrightarrows CO+H_2O \qquad \Delta H_{298\,K}=+41.21\ \text{kJ/mol} \tag{2}$$

$$CO_2+3H_2 \leftrightarrows CH_3OH+H_2O \qquad \Delta H_{298\,K}=-49.16\ \text{kJ/mol} \tag{3}$$

$$r_{CH_3OH,\,CO,\,1}=\frac{k_1K_{CO}\left[f_{CO}f_{H_2}^{1.5}-\frac{f_{CH_3OH}}{f_{H_2}^{0.5}K_1}\right]}{(1+K_{CO}f_{CO}+K_{CO_2}f_{CO_2})\left[f_{H_2}^{0.5}+\left(\frac{K_{H_2O}}{K_{H_2}^{0.5}}\right)f_{H_2O}\right]} \tag{4}$$

$$r_{H_2O,\,2}=\frac{k_2K_{CO_2}\left[f_{CO_2}f_{H_2}-\frac{f_{H_2O}f_{CO}}{K_2}\right]}{(1+K_{CO}f_{CO}+K_{CO_2}f_{CO_2})\left[f_{H_2}^{0.5}+\left(\frac{K_{H_2O}}{K_{H_2}^{0.5}}\right)f_{H_2O}\right]} \tag{5}$$

$$r_{CH_3OH,\,CO_2,\,3}=\frac{k_3K_{CO_2}\left[f_{CO}f_{H_2}^{1.5}-\frac{f_{CH_3OH}f_{H_2O}}{f_{H_2}^{1.5}K_3}\right]}{(1+K_{CO}f_{CO}+K_{CO_2}f_{CO_2})\left[f_{H_2}^{0.5}+\left(\frac{K_{H_2O}}{K_{H_2}^{0.5}}\right)f_{H_2O}\right]} \tag{6}$$

Table 3. Constants for driving force and chemical equilibrium data

Parameter	Value	Parameter	Value
K_{CO} [Pa^{-1}]	8.3965×10^{-11} exp (118,270/RT)	K_{CO_2}/K_2 [Pa^{-1}]	6.1221×10^{-13} exp (125,226/RT)
K_{CO_2} [Pa^{-1}]	1.7214×10^{-10} exp (81,287/RT)	K_{CO_2}/K_3 [Pa]	2.5813×10^{10} exp (26,788/RT)
K_{CO}/K_1 [Pa]	3.5408×10^{12} exp (19,832/RT)		

Table 4. K_i for adsorption term of Graaf's model

Term	Expression	a_i	b_i
1	1	1	0
2	$K_{H_2O}/K_{H_2}^{0.5}$	4.3676×10^{-12}	1.1508×10^{5}
3	K_{CO}	8.3965×10^{-11}	1.1827×10^{5}
4	$K_{CO}K_{H_2O}/K_{H_2}^{0.5}$	3.6673×10^{-22}	2.3335×10^{5}
5	K_{CO_2}	1.7214×10^{-10}	8.1287×10^{4}
6	$K_{CO_2}K_{H_2O}/K_{H_2}^{0.5}$	7.5184×10^{-22}	1.9727×10^{5}

where, $K_i=a_i\exp(b_i/RT)$

After methanol synthesis, the product from reactor (Stream 7 in Fig. 1) is cooled to 308 K using the feed of distillation column (DISTIL in Fig. 1) to save energy and separate the unreacted gas (10 in Fig. 1). The methanol-rich stream (Stream 9 in Fig. 1) is depressurized with adiabatic valve (V1) and heated to 360 K by the product stream of the methanol reactor, which is equal to the first distillation column (DISTIL in Fig. 1)'s feed condition [32]. Through the two-distillation column, water and CO_2 are separated from the methanol-rich stream, and as a result, 232 t/day of methanol having 99.4 wt% is produced. To increase the methanol production, the unreacted gas in flash drum and CO_2-rich stream (CO_2 in Fig. 1) are recycled to the feed stream. Before recycling the stream, 20 wt% of stream is purged to prevent the accumulation of product. However, the unreacted gas stream has a great deal of N_2 and H_2 flows due to the low conversion of methanol. To solve this unreacted gas problem, it is proposed to produce ammonia [33]. In this simulation, we used RGibbs reactor due to the lack of the reaction kinetics and we just describe conceptual design of ammonia process.

1-2. Process Description of Methanol-ammonia Coproduction Process

Fig. 2 shows the PFD of the co-production of methanol and ammonia using BFG from a steel manufacturing plant. Most of the process conditions, except feedstock and equipment condition, are equal to the methanol production case. Distillation section, such as reflux ratio and boil-up ratio of the distillation column, was adjusted due to the changed process, and feedstock was changed for fitting R=2. Ammonia synthesis was operated using Haber-Bosch process [24] at temperature 400 to 650 C and pressure 200 to 400 atm with catalyst [34]. Eq. (7) describes the reaction and the heat of reaction [35].

$$N_2+3H_2 \leftrightarrows 2NH_3 \qquad \Delta H_{298\,K}=-92.44\ \text{kJ/mol} \tag{7}$$

As shown in Eq. (7), as the ammonia reaction is highly exothermic, the optimal operating condition of the ammonia synthesis reactor (400 C, 200 bar) is selected using sensitivity analysis tool in ASPEN Plus simulator. In addition, CO and CO_2 need to be removed under 1 wt% from the unreacted gas stream at the flash drum in methanol section by pressure swing adsorption (PSA) process to prevent catalyst poisoning [25]. The PSA process is modelled with ASPEN Plus SEP model with 1 wt% separation [36,37], and the separated CO and CO_2 are recycled to methanol synthesis section to increase the methanol production.

Reactant stream (Stream SEPCO in Fig. 4) and recycled stream (Stream RE4 in Fig. 4) are mixed in mixer (MIX3) and passed through the three-stage multi-compressor with intercooling. After compression with intercooling, the feed stream (Stream S3 in Fig. 2) is to be 400 C and 200 bar, which is equal to ammonia reaction conditions. Then the reaction mixture (Stream RAW in Fig. 2) is cooled and depressurized to −30 C and 150 bar to maximize the product yield. The cooled stream (Stream COOLED in Fig. 2) is flashed at the adiabatic condition. The off-gas stream is re-heated to 20 C and 5 wt% of the off-gas is purged to prevent the accumulation of product, and the other is recycled to increase the ammonia production. Finally, 97.7 wt%, 453.4 t/day of ammonia and 99.8 wt%, 263 t/day of methanol are produced by the proposed process.

2. Economic Analysis

Economic feasibility studies, such as total annual capital cost (TAC) estimation, NPV analysis and sensitivity analysis, were based on the process simulation results. There are some assumptions in Table 5 [38].

2-1. CAPEX

The purchased costs for the equipment, excluding the ammonia, methanol reactor, HEN, multi-compressor and PSA modules are estimated using Aspen Process Economic Analyzer (APEA) V12. The cost of the methanol reactor is estimated using Eq. (8),

$$C_R=8,175\times D^{1.066}\times L^{0.802}\ (\$) \tag{8}$$

where L is the length and D is the diameter of the multi-tube Lurgi methanol reactor [21]. The specification of methanol reactor is obtained from the [30], which is described in Table 6.

The cost of ammonia reactor is obtained from study by Osman et al. [24]. The calculated ammonia reactor is US $392,100 when

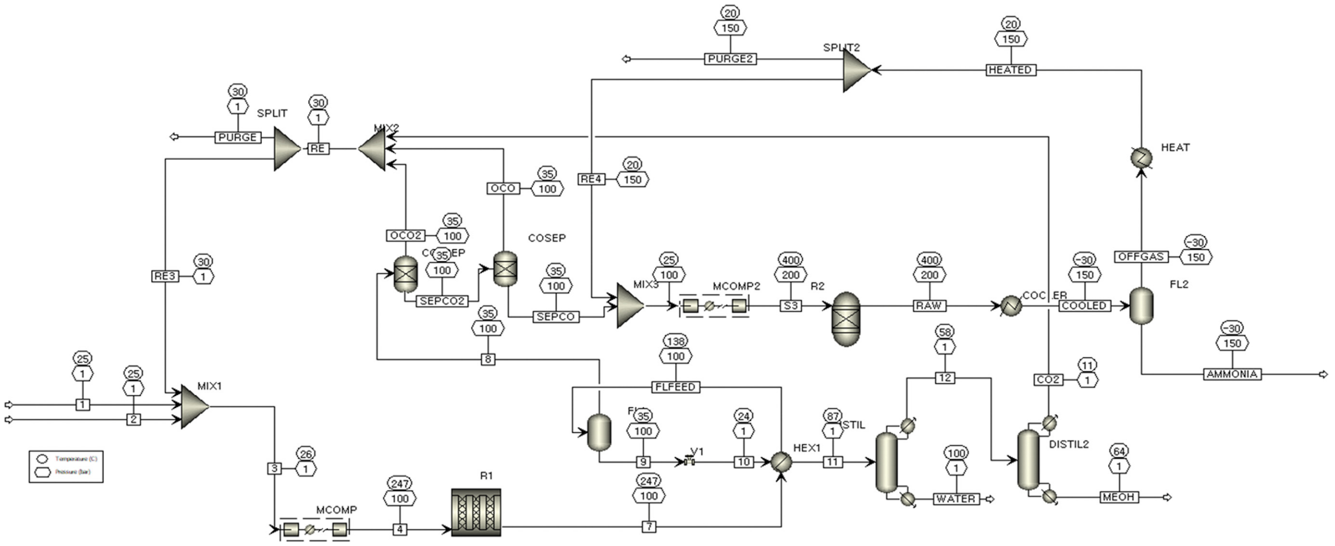

Fig. 2. The PFD of co-production of NH_3 and methanol.

Table 5. Economic assumptions in this study

Economic assumption	Value
1. Project life	20 years
2. Plant uptime	350 days/y
3. Construction period & capital distribution	3 years (1st year: 15%, 2nd year: 35%, 3rd year: 50%)
4. Construction inflation rate	2% per year
5. On stream factor of each year	1st year: 50% 2nd year: 90%, 3rd year~ end year: 100%
6. Income tax rate	10% of Fixed capital investment (FCI) [39]
7. Plant location	U.S. Gulf
8. Base year	2018 (CEPCI: 603.1) (we assumed)
9. Discount rate	7%
10. Startup cost	10% of FCI [39]
11. Depreciation	None (we assumed)
12. Methanol, ammonia selling price	470 \$/t (methanol) [47], 514 \$/t (ammonia) [48]

Table 6. Specification of methanol reactor

Parameter	Value
Tube length	7.022 m
Tube diameter	38 mm
Number of tubes	2,962
Bed voidage	0.39
Particle density	1,132 kg/m^3
Inlet flow rate	0.64 mol/s

the mass flow rate is 416,000 kg/hr. But in our study, the feed mass flow rate was 32,475 kg/hr. So, we applied the most common simple relationship between the purchased cost and an attribute of the equipment related to units of capacity, six-tenth rule which is described in Eq. (9),

$$\frac{C_a}{C_b} = \left(\frac{A_a}{A_b}\right)^n \tag{9}$$

where A is the equipment cost attribute, C is purchased cost, n is cost exponent, a is equipment with the required attribute and b is equipment with the base attribute, respectively [40].

The cost of the HEN was calculated by using Eq. (10), which is based on the bare module cost method [40].

$$C_{BM}=C_p^o[B_1+B_2F_PF_M] \tag{10}$$

F_P can be calculated by Eq. (11), and F_M=2.7 for stainless steel and 1 for carbon steel.

$$\log_{10}F_p=C_1+C_2\log_{10}P+C_3(\log_{10}P)^2 \tag{11}$$

where P is the pressure of the HEN as a unit of barg. The heater and cooler in the ammonia section are selected with spiral tube with stainless shell and tube for which the allowable pressure ($P<150$ barg) was satisfied. So, the $C_1=C_2=C_3=0$, $B_1=1.74$ and $B_2=1.55$. The heat transfer area for heater and cooler in ammonia section is assumed as 100 m^2 and the bare module cost is obtained by Eq. (9). This equation is based on the year 2001, considering inflation over time. So, the calculated bare module cost can be adjusted by Eq. (12) [40].

$$C_{2018}=C_{BM(2001)}\left(\frac{I_{2018}}{I_{2001}}\right)\ (\$) \tag{12}$$

The I is the year of the chemical plant cost index (CEPCI), the CEPCI in 2018 is 603.1 and the CEPCI of 2001 is 397 [41].

The multi-compressor cost is estimated by the summation of each compressor and intercooler. The compressor cost was calculated by Eq. (13)-(14) [42],

$$C_P=F_DF_MC_B\ (\$) \tag{13}$$

$$C_B=\exp\{9.1553+0.63[\ln(P_C)]\} \tag{14}$$

where F_D=1.25 for gas turbine drive, F_M=2.5 for stainless steel and P_C is the horsepower of compressor.

The intercooler cost for methanol section was estimated with Eq. (10) where $F_M=1$, $B_1=1.63$ and $B_2=1.66$ and heat exchange area is 100 m^2. The pressure of intercooler in the methanol section is met under the allowable pressure for floating-head type heat exchanger ($P<100$ barg), while the pressure of intercooler in the ammonia section is over 100 barg; it can be calculated with the spiral tube type similar to heater and cooler.

The PSA modules were estimated by Eq. (15),

$$C_{PSA}=6{,}242\times f/21{,}257.6\ (\text{K}\$) \tag{15}$$

where f is the volumetric flow of the feedstock in Nm^3/h [42]. The other equipment cost that APEA cannot calculate, such as mixer, valve and splitter, was ignored in this study.

The total capital cost is defined as the sum of fixed capital investment (FCI) and working capital. The FCI is the sum of the direct cost (i.e., equipment installation, building and building services, yard improvement), land cost and indirect cost (i.e., engineering, construction expenses, contractor's fee, contingency). All the components of total capital cost were based on the percentage of the FCI that obtained from [40]. The percentage of these components is described in Table 7.

2-2. OPEX

To calculate the total operating cost (TOC), the raw material costs of BFG and H_2 cost are needed. The cost of BFG is obtained from dividing the 2018 average natural gas cost based on Henry Hub price [43] by its LHV [44]. The cost of H_2 is obtained from the interpolation between the cost of 2015 DOE target and 2020 DOE

Table 7. CAPEX percentage distribution

Component	Percentage
Equipment cost	25% FCI
Equipment installation	10% FCI
Buildings and building services	10% FCI
Yard improvement	5% FCI
Service facilities	15% FCI
Land	2% FCI
Engineering	10% FCI
Construction expenses	10% FCI
Contractor's fee	4% FCI
Contingency	10% FCI
Working capital	15% TCI

Table 8. OPEX percentage distribution

Component	Percentage
Raw material cost	-
Utility cost	15% TOC
Operating labor	10% TOC
Maintenance and repair	10% FCI
Local taxes	2% FCI
Insurance	0.6% FCI
Plant overhead	10% TOC
Others	5% FCI

target, that is 2.94 $/kgH$_2$. Utility costs for each equipment except methanol, ammonia reactor, cooler and heater in ammonia section are calculated with APEA. Their utility costs are calculated with the specific setting of ASPEN Plus utility. When cooling is required in methanol, ammonia reactor and cooler in the ammonia section, cooling water is the appropriate utility to cool this equipment. Also, heating is required in the heater in the ammonia section, steam is the appropriate utility to heat this equipment. Unit utility costs such as electricity (0.0775 $/kWh), cooling water ($2.12*10^{-7}$ $/kJ), steam ($1.9*10^{-6}$ $/kJ), and refrigerant ($3.36*10^{-6}$ $/kJ) are set as the default values in APEA. Operating labor, maintenance and repair, insurance and plant overhead are estimated based on the percentage of the total operating cost. The percentage of these components is also described in Table 8 [39].

We calculated total annual capital cost (TACC) to estimate the current cost of annuity [45] and cost distribution of the total annual cost. To calculate the total annual capital cost, a capital recovery factor (CRF) was employed as described in Eq. (16),

$$\mathrm{CRF} = \frac{\mathrm{i}(1+\mathrm{i})^{n}}{(1+\mathrm{i})^{n}-1} \tag{16}$$

where i is the discount rate, n is the project lifecycle. The annual capital cost is defined the product of CRF and capital cost (CRF=0.0943).

To find the profitability, we calculated the NPV with discounted cash flow method defined in Eq. (17),

$$\mathrm{NPV} = \Sigma_{i=1}^{n}\frac{\mathrm{CF}_i}{(1+\mathrm{r})^{i}} - \mathrm{C}_{inv} \tag{17}$$

where CF$_i$ is the cash flow generated in the ith year in $, calculated as the difference between the total revenue and the cost of operation and maintenance, n is the lifetime of the project, r is the annual discount rate and C$_{inv}$ is the cost of the investment [46]. If the NPV is positive, the project is profitable and attractive for investment, while a negative value indicates the project is defective and unattractive for investment. The selling prices of the methanol and ammonia are given in Table 5.

RESULTS AND DISCUSSION

1. Process Simulation Result

This study developed a combined production method of methanol and ammonia from BFG over Cu/ZnO/Al$_2$O$_3$ catalysts for methanol reactor and Fe catalyst for ammonia reactor. For each case the molar flow rate of H$_2$ was adjusted to fit the R parameter equals 2.55 t/day of H$_2$ was fed in the base case, while 132.1 t/day of H$_2$ was fed in the proposed case. The key stream data for all cases are shown in Table S1 and S2 in Supplementary Information.

In the only methanol production case, BFG (775 t/day), H$_2$ and recycle stream (2,189 t/day) are mixed and pressurized through multi-compressor to 100 bar, 520 K. Then, the pressurized stream is fed to 28.2% molar yield reactor following Graaf's kinetic models. After the reaction, 61 wt% of N$_2$, 22 wt% of CO$_2$, 2 wt% of CO, 1 wt% of H$_2$O and 8 wt% of methanol are produced and cooled to 308 K to separate the unreacted gas. In the flash drum, 99 wt% of the N$_2$, H$_2$, CO, and CO$_2$ is flashed and sent to the second mixer, and 62 wt% of liquid methanol stream is depressurized in the adiabatic valve and heated to 87 °C with the product stream of methanol reactor. The water is separated from the heated stream in the first 30 stage distillation column and sent to the wastewater treatment facility. Top product from the previous column is fed to the second 30 stage distillation column, 99.4 wt%, 232 t/day of methanol is obtained from the bottom of the column at 337 K, 1 bar.

In the proposed case producing methanol and ammonia simultaneously, the methanol subsystem is almost the same as the base case, while the feed rate of H$_2$ (132 t/day) and production rate of methanol (99.8 wt%, 263 t/day) are different from the base for fitting the R=2. The unreacted gas in the flash drum is fed to PSA modules to separate CO$_2$ (409 t/day) and CO (41 t/day) to prevent catalyst poisoning. The separated gas is mixed with the top product of second distillation column in methanol section and 20 wt% (110 t/day) is purged to prevent the accumulation of the product. The CO$_2$ and CO separated stream (470 t/day) is mixed with the recycled stream (310 t/day) and pressurized through the multi-compressor to 200 bar. Then, the pressurized stream is cooled to 400 °C and sent to a 13.8% molar yield reactor. As a result, 59 wt% of ammonia stream is produced and refrigerated to −30 °C to separate the unreacted gas and ammonia. Finally, 98 wt%, 453 t/day of ammonia is produced from the flash drum at −30 °C, 150 bar. The unreacted gas is heated to 20 °C and 5 wt% of the gas is purged to prevent the accumulation of unreacted gas.

2. Heat Integration

Heat integration is conducted using Aspen Energy Analyzer (AEA) to minimize the utility usage of the whole process. We assumed that the minimum allowable temperature difference is 10 K,

Table 9. The energy requirement of each cases

	Base case		Proposed case	
	Before	After	Before	After
Heating (MW)	21.6	6.95	19.82	0.00
Cooling (MW)	30.49	15.83	69.89	50.01
Total	52.09	22.78	89.71	50.01

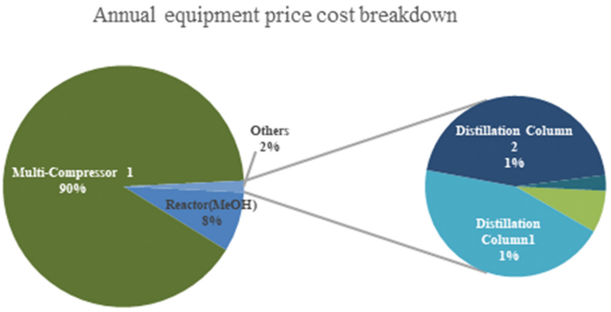

Fig. 3. Equipment cost distribution chart at the base.

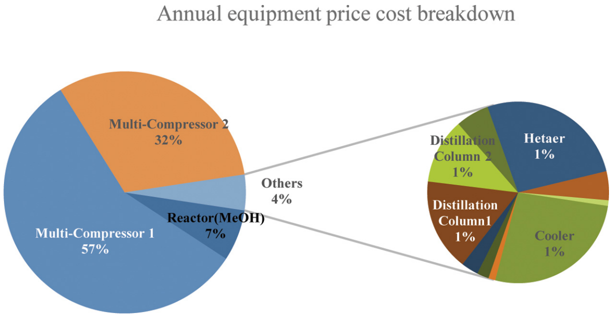

Fig. 4. Equipment cost distribution chart at the proposed case.

which is the minimum pinch point of the heat exchange network (HEN). The feasible heat exchange area was determined by the minimum heating and cooling requirements [49].

We performed heat integration to save the energy requirement of heating and cooling utility. The summary of the heat integration is described in Table 9. In the only methanol production case, 21.6 MW of heating and 30.49 MW of cooling utility were required to operate the whole process. Heating energy was only used in methanol reactor. After the heat integration, 6.95 MW of heating and 15.83 MW of cooling utility were reduced, respectively. That is, the total utility is 56.3% reduced when performing the heat integration.

In the proposed case, 19.82 MW of heating and 69.89 MW of cooling utility were required. Compared to the case producing only methanol, the heating requirement increased because the feed of H_2 in the methanol reactor was increased to fit the R=2 and reheat the recycle flow. According to the increase of H_2 molar flow, the cooling requirement is also increased. After heat integration, no heating energy was required and 50.01 MW of cooling utility was reduced, respectively. That is, the total utility was 44.3 % reduced by the heat integration.

3. Economic Analysis

Figs. 3-5 show the main components of the total annual equipment cost and total capital cost distribution for each case. The equipment cost is calculated by APEA except the multi-compressors, methanol/ammonia reactor and heat exchangers. The percentages of the total capital cost are estimated by Peters et al. [39].

The calculated TACC was US 29.8 M$/y in the only methanol production case and US 34.9 M$/y in the methanol/ammonia coproduction case. In both cases, the multi-compressor in the methanol section is the major component of the TACC. The second major component of TACC is a methanol reactor at the only methanol production case and multi-compressor in the ammonia section at the proposed case. The difference of the TACC was because the amount of the energy was different due to the addition of equipment for ammonia synthesis (US 2.55 M$/y) and the increase in the supply of hydrogen.

The calculated TOC was US 91.8 M$/y at the only methanol production case and 187.10 M$/y at the proposed case. The raw material cost for all cases was the major component (56.6 M$/y at the base case, US 135.9 M$/y at the proposed case) in this study.

The difference (US 79.3 M$/y) occurred because of the increase

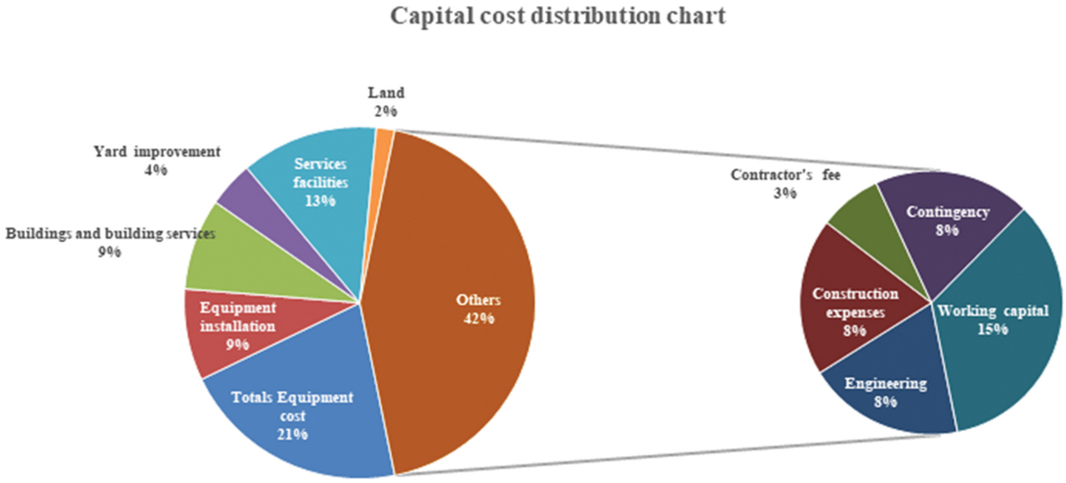

Fig. 5. Annual capital cost distribution chart for all cases.

Table 10. Utility usage for each equipment in this study

Equipment	Type	Cost	
		Base ($/hr)	Propose ($/hr)
Multi-Compressor (methanol)	Electricity	2,868.65	2,868.65
Reactor (methanol)	Cooling water	5.30	5.95
Flash Tank 1(methanol)	Cooling water	8.66	5.04
Distillation Column 1 (methanol)	Cooling water, LP steam	147.01	76.52
Distillation Column 2 (methanol)	Refrigerant, LP steam	202.66	59.12
Multi-Compressor (NH_3)	Electricity	-	488.45
Reactor (NH_3)	Cooling water	-	12.04
Cooler (NH_3)	Refrigerant	-	392.51
Flash Tank 2 (NH_3)	None (Adiabatic)	-	-
Heater	LP steam	-	15.57

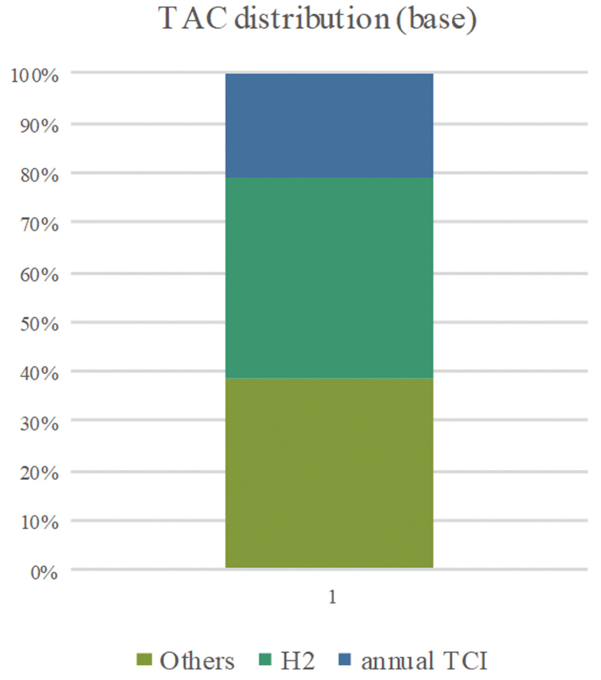

Fig. 6. TAC distribution chart for base case.

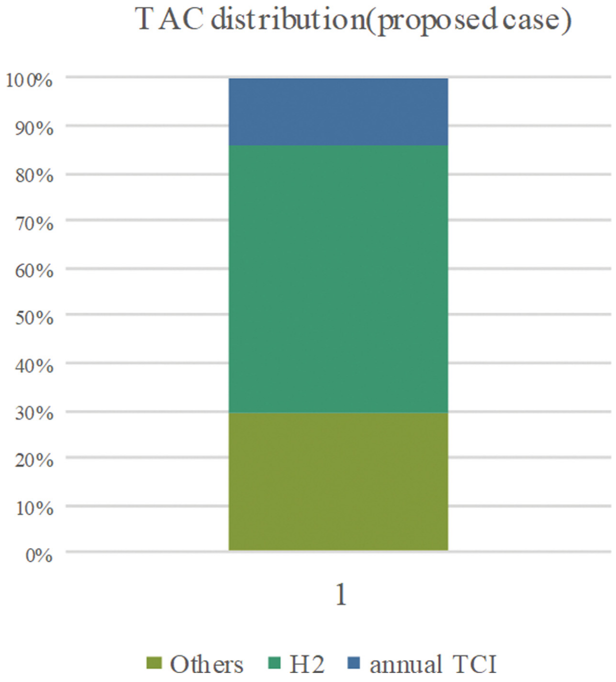

Fig. 7. TAC distribution chart for proposed case.

in the H_2 molar flow rate in the proposed case. The utility costs calculated by APEA were described in Table 10. It shows the utility type and usage of each component except PSA module.

The TAC we calculated was US 121.6 M$/y for the base and US 222.1 M$/y for the proposed case. The TAC distribution (TACC, H_2 cost, other operating costs) charts for each case were described in Fig. 6 and 7. As can be seen from the figure, the cost of the H_2 production accounted for over 40% for all cases.

The $N_2:H_2$ molar flow rate did not fit the stoichiometry, 1 : 3. In order to fit the stoichiometry, 44,062.2 kmol/day of make-up N_2 from the air was needed, respectively.

But makeup N_2 causes the increase of the energy requirement of the multi-compressor, ammonia reactor and cooler in the ammonia synthesis section, so those results cause capital and operating cost increases and degraded molar purity. So, the feed $N_2:H_2$ ratio is the same as the flash drum in the methanol section 1 : 12.4 and no additional supply chain of the N_2 was set.

The estimated NPV is US −810.4 M$ at the base and US −981.3 M$ at the proposed case so the difference between two cases is US 171 M$. All the cases are shown economically infeasible because the selling prices of methanol (US 470 $/t) and ammonia (US 514 $/t) are lower than the H_2 production cost (US 2,940 $/t). Also, the total revenues of methanol (US 38.1 M$/y at the base case, US 43.0 M$/y at the proposed case) and ammonia (US 81.6 M$/y) do not exceed the raw material cost for every year. So, it results in a decrease of the present value as the years go by and get negative NPV. Comparing the two cases, the methanol/ammonia coproduction process is less economically feasible than the only methanol production process. It is because of the increase of the H_2 molar flow rate to fit the R parameter and it results in the increase of the energy requirement and operating cost. Also, the ammonia synthesis is an energy intensive process due to the low N_2 reactiv-

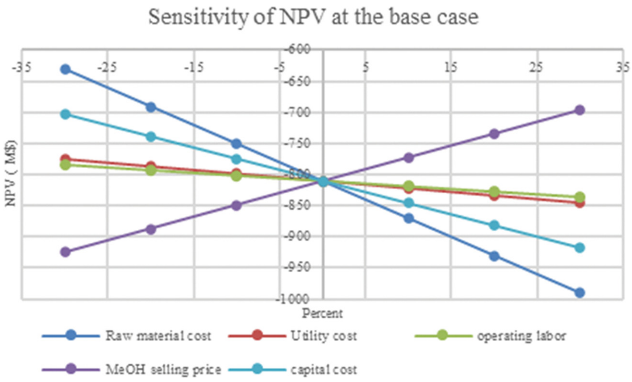

Fig. 8. The result of sensitivity of NPV at the base.

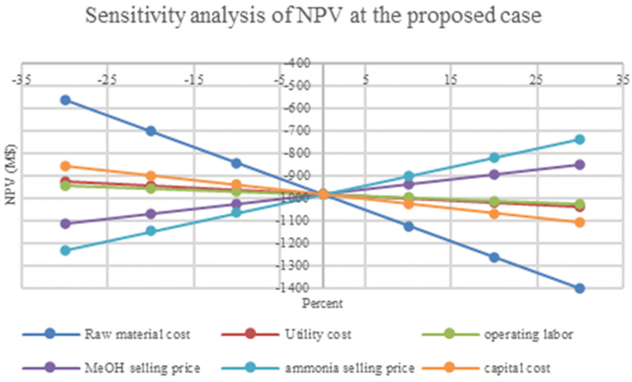

Fig. 9. The result of sensitivity of NPV at the proposed case.

ity and requires high temperature and low pressure. Furthermore, as shown in Eq. (7), it is a highly exothermic reaction, increases utility usage and cost.

4. Sensitivity Analysis

Sensitivity analysis is performed to show the variability of NPV as a function of the economic parameters for all cases (i.e., H_2 production cost, utility cost, discount rate, capital cost and products selling price such as methanol and ammonia). One of the economic parameters is adjusted within the range of –30 to 30 percent, while other parameters are kept constant. The results of sensitivity analysis are shown in Figs. 8-9.

In the only methanol production case, as shown in Fig. 8, NPV is the most sensitive to the raw material cost, especially H_2 cost, followed by methanol selling price and capital cost. The highest NPV is US −630.9 M$ and the lowest NPV is US −989.9 M$. When the raw material cost decreases −30%, the NPV increases 22.1% and the methanol selling price is increased and capital cost is decreased by 30% each, the NPV increases 13.2% each. The impact on the NPV by changing the utility and operating labor is relatively small (6.0% and 5.1%).

In the proposed case, NPV is the most sensitive to the raw material cost (same as base case) followed by ammonia selling price, methanol selling price and capital cost. The highest NPV is US −562.8 M$ and the lowest NPV is US −1,399.8 M$. When the raw material cost decreases −30%, the NPV increases 42.6% and the ammonia and methanol selling price increases by 30% each, the NPV increases 13.2%, 25.0% each. The impact on the NPV by changing the utility and operating labor is similar with the base case (5.7% and 4.0% each).

The NPV variation when changing the discount rate for the only methanol production case is US −699.4 M$ to US −970.5 M$ and the proposed case is US −852.0 M$ to US −1,167.9 M$ changing the discount rate from 4% to 10%.

Comparing the two cases in terms of the variation of the NPV, when raw material cost decreases 30%, the case we proposed is more economically feasible than the base case. The NPV of the only methanol production case is US −630.9 M$ and proposed case is US −562.8 M$, so the proposed method is more economically feasible by US 68.1 M$. This is due to the higher production of methanol and ammonia with more feedstock of H_2. Although the difference of NPV is not significant, it is noteworthy that combining the two different cases (methanol, ammonia) can be more profitable than the base case.

CONCLUSION

This study proposes a promising CCU technology for producing the high-value chemicals methanol and ammonia simultaneously from the mixed feed of BFG made from steel manufacturing plant and H_2 produced by water electrolysis. The proposed methanol and ammonia coproduction process is compared to the conventional one producing only methanol. Methanol synthesis is based on the previous experimental study of reaction kinetics using CO and CO_2 over a commercial $Cu/ZnO/Al_2O_3$ catalyst. From the simulation results, the proposed process can produce the 99.8 wt%, 263 t/day of methanol and 98 wt%, 453 t/day of ammonia simultaneously, while the only methanol production case produces 99.4 wt%, 232 t/day of methanol.

In both cases, heat integration was performed with AEA V12. After the heat integration, the total utility consumption decreased 56.3% at the base case and 44.3% for the proposed case.

To analyze the economic feasibility, we assumed economic parameters such as project lifetime, operational day and discount rate based on the previous studies. Equipment cost and utility cost were determined by APEA, and other components were determined by the percentage of FCI or total operating cost. To determine profitability, we estimated the NPV of both cases. The NPV of base case was −810.4 M$, while the proposed case was −981.3 M$. Thus, it can be concluded that there is no profitability for all cases due to the negative values of NPV. Furthermore, the proposed case is less profitable than the only methanol production case because the high pressure and temperature of ammonia synthesis and considerable energy requirements.

Sensitivity analysis was performed to examine the NPV of this process with respect to variations in economic parameters such as the raw material cost, products selling price and capital cost. We changed each parameter from −30% to 30% and got a result of the variation of NPV. The NPV changed from US −989.9 M$ to US −630.8 M$ when adjusting the raw material cost in the base case, and US −1,399.8 M$ to US −562.8 M$ when adjusting the raw material cost in the proposed case. It is found that if the raw material cost decreased 30%, the proposed case was more economically feasible than the base case at the point of the NPV. As a conclusion, all the cases can be economically feasible when the methanol selling price is over four times more than the current, ammonia selling price is over two times more than the current, and the hydrogen production cost is decreased over 80%. A lower H_2 production cost and higher market price of methanol and ammonia would be a potential to develop this CCU technology.

ACKNOWLEDGEMENTS

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NOMENCLATURE

IEA : international energy agency
COG : coke oven gas
BOFG : basic oxygen furnace gas
BFG : blast furnace gas
CCS : carbon capture & storage
CCU : carbon capture & utilization
LHV : lower heating value
DME : dimethyl ether
SMR : steam methane reforming
CAGR : compound annual growth rate
PFD : process flow diagram
PSA : pressure swing adsorption
TAC : total annual cost
TACC : total annual capital cost
TOC : total operating cost
NPV : net present value
HEN : heat exchanger network
AEA : aspen energy analyzer
APEA : aspen process economic analyzer
FCI : fixed capital investment
CRF : capital recovery factor
CAPEX : capital expenditure
OPEX : operating expenditure
wt : weight

SUPPORTING INFORMATION

Additional information as noted in the text. This information is available via the Internet at http://www.springer.com/chemistry/journal/11814.

REFERENCES

1. IEA, Global Energy & CO2 Status Report 2019, IEA, Paris (2019).
2. D. C. Rosenfeld and M. Lehner, *Renew. Energy*, **147**, 1511 (2020).
3. W. Liu and F. Yang, *Int. J. Hydrog. Energy*, **46**, 10548 (2021).
4. P. Cavaliere, *Clean ironmaking and steelmaking processes*, Springer, Lecce, Italy (2019).
5. K. Jiang, P. Ashworth and D. Angus, *Renew. Sust. Energ. Rev.*, **119**, 109601 (2020).
6. G. Leonzio, *J. CO_2 Util.*, **27**, 326 (2018).
7. A. H. Tamboli and H. Kim, *Chem. Eng. J.*, **323**, 530 (2017).
8. J. Artz and W. Leitner, *Chem. Rev.*, **118**, 434 (2018).
9. R. M. Cuéllar-Franca and A. Azapagic, *J. CO_2 Util.*, **9**, 82 (2015).
10. J. K. Lee, I. B. Lee and J. Han, *J. Ind. Eng. Chem.*, **75**, 77 (2019).
11. W. H. Chen and S. W. Du, *Energy*, **86**, 758 (2015).
12. W. U. Soto and L. Falk, *Renew. Sustain. Energy Rev.*, **74**, 809 (2017).
13. W. Zheng and W. Zeng, *Fuel*, **302**, 121100 (2021).
14. GlobeNewswire, https://www.globenewswire.com/news-release/2021/06/25/2253193/28124/en/Global-Methanol-Market-2021-to-2026-Industry-Trends-Share-Size-Growth-Opportunity-and-Forecasts.html (2021).
15. Methanol institute, https://www.methanol.org/methanol-price-supply-demand/ (2021).
16. B. Lee and H. Lim, *Appl. Energy*, **279**, 115827 (2020).
17. M. P. Fortes and E. Tzimas, *Appl. Energy*, **161**, 718 (2016).
18. S. Shin and I. B. Lee, *Energy*, **200**, 117506 (2020).
19. N. Meunier and G. D. Weireld, *Renew. Energy*, **146**, 1192 (2020).
20. J. M. Bermúdez and J. A. Menéndez, *Fuel*, **89**, 2897 (2010).
21. D. Kim and J. Han, *Energy*, **198**, 117355 (2020).
22. U.S. Geological Survey, Mineral Commodity Summaries 2019, Reston, VA, USA (2019).
23. Grand View Research, https://www.grandviewresearch.com/industry-analysis/ammonia-market (2017).
24. O. Osman and A. Sleptchenko, *J. Clean. Prod.*, **271**, 121627 (2020).
25. E. Koohestanian and A. Samimi, *Energy*, **144**, 279 (2018).
26. N. D. Pawar and D. Stolten, *Int. J. Hydrog. Energy*, **46**, 27247 (2021).
27. AspenTech$^{®}$, https://lms.nchu.edu.tw/sysdata/doc/1/196bb4d4fac4c3d7/pdf.pdf (2018).
28. H. A. Kalbani and H. Wang, *Appl. Energy*, **165**, 809 (2016).
29. M. Matzen and Y. Demirel, *Energy*, **93**, 1 (2015).
30. A. Alarifi and E. Croiset, *Ind. Eng. Chem. Res.*, **55**, 1164 (2016).
31. G. H. Graaf, E. J. Stamhuis and A. A. C. M. Beenackers, *Chem. Eng. Sci.*, **43**, 3185 (1988).
32. J. Nyári and A. S. Aarnio, *J. CO_2 Util.*, **39**, 101106 (2020).
33. P. L. Spath and D. C. Dayton, NREL, Golden (CO, USA) (2003).
34. Encyclopedia Britannica, https://www.britannica.com/technology/Haber-Bosch-process (2020).
35. L. J. Christiansen, *Ammonia: Catalysis and manufacture*, Springer-Verlag, Lyngby, Denmark (1995).
36. Y. I. Lim, J. Choi, H. M. Moon and G. Kim, *Korean Chem. Eng. Res.*, **54**, 3 (2016).
37. D. M. Ruthven, S. Farooq and K. S. Knaebel, *Pressure swing adsorption*, Wiley, New York, USA (1994).
38. C. Zhang and S. C. Kang, *Fuel*, **157**, 285 (2015).
39. M. S. Peters, K. Timmerhaus and R. West, *Plant design and economics for chemical engineers*, McGraw-Hill Professional, New York, USA (2002).
40. R. A. Turton, *Analysis, synthesis, and design of chemical processes*, Prentice Hall, Hoboken, New Jersey, USA (2003).
41. Chemical engineering, https://www.chemengonline.com (2021).
42. W. D. Seider and J. D. Seader, *Product and process design principles*, Wiley, New York, USA (2010).

43. The Engineering ToolBox, https://www.engineeringtoolbox.com/fuels-higher-calorific-values-d_169.html (2021).
44. METGroup, https://group.met.com/en/media/energy-insight/calorific-value-of-natural-gas (2021).
45. A. Ebrahimi and M. Ziabasharhagh, *Energy*, **126**, 868 (2017).
46. F. P. Alege and P. M. Ndegwa, *J. Clean. Prod.*, **310**, 127481 (2021).
47. D. Bellotti and L. Magistri, *Energy Procedia*, **158**, 4721 (2019).
48. G. Schnitkey, Weekly Farm Economics. 178 (2018).
49. J. M. Douglas, *Conceptual design of chemical processes*, McGraw-Hill New York, USA (1988).

Supporting Information

Techno-economic analysis of methanol and ammonia co-producing process using CO_2 from blast furnace gas

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A. Key Stream Data

Table S1. Key stream data for methanol production case

Stream name	Units	1	2	4	7
Description					
From				MCOMP	R1
To		MIX1	MIX1	R1	HEX1
Phase		Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase
Temperature	C	25	25	31.25184722	246.85
Pressure	bar	1	1	1	100
Molar Vapor Fraction		1	1	1	1
Molar Liquid Fraction		0	0	0	0
Mole Flows	kmol/hr	1,136.807085	1,048.922286	6,823.529708	6,217.71845
CO	kmol/hr	0	208.2559811	312.0020637	129.6902095
H_2O	kmol/hr	0	0	0.735101614	121.3288764
CH_3OH	kmol/hr	0	0	11.4159883	314.3216173
H_2	kmol/hr	1,136.807085	41.33843946	2,985.19617	2,258.791137
CO_2	kmol/hr	0	248.9975717	762.5289168	641.9351421
N_2	kmol/hr	0	550.3302935	2,751.651467	2,751.651467

Stream name	Units	9	10	13	MEOH
Description					
From		FL1	FL1	DISTIL	DISTIL2
To		V1	MIX2	DISTIL2	
Phase		Liquid Phase	Vapor Phase	Vapor Phase	Liquid Phase
Temperature	C	34.85	34.85	57.76036114	64.34800934
Pressure	bar	100	100	1	1
Molar Vapor Fraction		0	1	1	0
Molar Liquid Fraction		1	0	0	1
Mole Flows	kmol/hr	523.1705806	5,694.547855	405.6983195	302.9904488
CO	kmol/hr	1.269629113	128.4205802	1.269629113	1.11303E-50
H_2O	kmol/hr	120.4100398	0.918836735	2.937778656	2.937778627
CH_3OH	kmol/hr	304.7479878	9.573629001	304.7479878	300.0526702
H_2	kmol/hr	1.539636613	2,257.2515	1.539636613	1.0439E-68
CO_2	kmol/hr	70.08394932	571.8511833	70.08394932	4.994E-33
N_2	kmol/hr	25.119338	2,726.532126	25.119338	8.25407E-50

Stream name	Units	RAW	RE
Description			
From		V1	SPLIT
To		HEX1	MIX1
Phase			Vapor Phase
Temperature	C	23.97841711	34.1884779
Pressure	bar	1	1
Molar Vapor Fraction		0.204451535	1
Molar Liquid Fraction		0.795548465	0
Mole Flows	kmol/hr	523.1705806	4,637.800337
CO	kmol/hr	1.269629113	103.7460826
H_2O	kmol/hr	120.4100398	0.735101614
CH_3OH	kmol/hr	304.7479878	11.4159883
H_2	kmol/hr	1.539636613	1,807.050645
CO_2	kmol/hr	70.08394932	513.5313452
N_2	kmol/hr	25.119338	2,201.321174

Table S2. Key stream data for co-production case

Stream name	Units	1	2	4	7
Description					
From				MCOMP	R1
To		MIX1	MIX1	R1	HEX1
Phase		Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase
Temperature	C	25	25	246.85	246.85
Pressure	bar	1	1	100	100
Molar Vapor Fraction		1	1	1	1
Molar Liquid Fraction		0	0	0	0
Mole Flows	kmol/hr	2,730	1,048.922286	4,226.499422	3,532.15448
CO	kmol/hr	0	208.2559811	259.2905526	64.41626336
H_2O	kmol/hr	0	0	2.26736E-08	152.2981817
CH_3OH	kmol/hr	0	0	6.873676536	354.0461475
H_2	kmol/hr	2,730	41.33843946	2,779.021322	1,932.378198
CO_2	kmol/hr	0	248.9975717	620.1373363	467.8391547
N_2	kmol/hr	0	550.3302935	561.1765345	561.1765345
AMMONIA	kmol/hr	0	0	0	0

Stream name	Units	8	9	10	12
Description					
From		FL1	FL1	V1	DISTIL
To		CO2SEP	V1	HEX1	DISTIL2
Phase		Vapor Phase	Liquid Phase		Vapor Phase
Temperature	C	34.85	34.85	24.15973133	58.06002059
Pressure	bar	100	100	1	1
Molar Vapor Fraction		1	0	0.186442262	1
Molar Liquid Fraction		0	1	0.813557738	0
Mole Flows	kmol/hr	2,929.628107	602.5276588	602.5276588	452.1044232
CO	kmol/hr	62.33474528	2.081529462	2.081529462	2.081529462
H_2O	kmol/hr	0.579602576	151.7181126	151.7181126	1.294877035
CH_3OH	kmol/hr	4.772546441	349.2750897	349.2750897	349.2750897
H_2	kmol/hr	1,922.77466	9.603557438	9.603557438	9.603557438
CO_2	kmol/hr	391.5477729	76.29159962	76.29159962	76.29159962
N_2	kmol/hr	547.61878	13.5577699	13.5577699	13.5577699
AMMONIA	kmol/hr	0	0	0	0

Stream name	Units	AMMONIA	FLFEED	MEOH	OFFGAS
Description					
From		FL2	HEX1	DISTIL2	FL2
To			FL1		HEAT
Phase		Liquid Phase		Liquid Phase	Vapor Phase
Temperature	C	−29.99999909	138.1856974	64.25811613	−29.99999909
Pressure	bar	150	100	1	150
Molar Vapor Fraction		0	0.929676958	0	1
Molar Liquid Fraction		1	0.070323042	1	0
Mole Flows	kmol/hr	1,107.367365	3,532.15448	341.9780559	5,730.024892
CO	kmol/hr	0.329313119	64.41626336	6.73435E-49	5.87957337
H_2O	kmol/hr	0.579602562	152.2981817	1.294877007	2.74371E-07
CH_3OH	kmol/hr	4.772526786	354.0461475	340.6831789	0.000392476
H_2	kmol/hr	11.53725519	1,932.378198	6.21792E-66	5,633.962714
CO_2	kmol/hr	3.825874316	467.8391547	2.23685E-33	1.790233113
N_2	kmol/hr	2.320061036	561.1765345	1.08763E-48	43.59160588
AMMONIA	kmol/hr	1,084.002732	0	0	44.80037303

Stream name	Units	RAW	RE3	RE4	S3
Description					
From		R2	SPLIT	SPLIT2	MCOMP2
To		COOLER	MIX1	MIX3	R2
Phase		Vapor Phase	Vapor Phase	Vapor Phase	Vapor Phase
Temperature	C	400	30.29824484	20	400
Pressure	bar	200	1	150	200.0000041
Molar Vapor Fraction		1	1	1	1
Molar Liquid Fraction		0	0	0	0
Mole Flows	kmol/hr	6,837.392257	447.5771362	5,443.353937	7,923.638351
CO	kmol/hr	6.208886489	51.03457153	5.585539036	6.208886489
H_2O	kmol/hr	0.579602837	2.26736E-08	2.6063E-07	0.579602837
CH_3OH	kmol/hr	4.772919262	6.873676536	0.000372822	4.772919262
H_2	kmol/hr	5,645.499969	7.682882499	5,352.094451	7,274.869111
CO_2	kmol/hr	5.61610743	371.1397647	1.700629701	5.61610743
N_2	kmol/hr	45.91166691	10.84624097	41.415934	589.034714
AMMONIA	kmol/hr	1,128.803105	0	42.55701087	42.55701087

Stream name	Units	SEPCO	SEPCO2
Description			
From		COSEP	CO2SEP
To		MIX3	COSEP
Phase			
Temperature	C	34.85	34.85
Pressure	bar	100	100
Molar Vapor Fraction		0.999947675	0.999979798
Molar Liquid Fraction		5.23247E-05	2.0202E-05
Mole Flows	kmol/hr	2,480.284414	2,541.995812
CO	kmol/hr	0.623347453	62.33474528
H_2O	kmol/hr	0.579602576	0.579602576
CH_3OH	kmol/hr	4.772546441	4.772546441
H_2	kmol/hr	1,922.77466	1,922.77466
CO_2	kmol/hr	3.915477729	3.915477729
N_2	kmol/hr	547.61878	547.61878
AMMONIA	kmol/hr	0	0