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Towards low-carbon ammonia: simulation and economic evaluation of blue ammonia with carbon utilization

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Abstract
The proposed blue ammonia production considers technical, environmental, and economic aspects. The design of the blue ammonia using CCUS (Carbon Capture, Utilization, and Storage) technology in this study contributes to reducing carbon emissions and providing a more environmentally friendly ammonia supply in East Java, Indonesia, due to the availability of raw materials and geological storage locations for CO_2 storage. Technically, the blue ammonia production was simulated with Aspen Hysys V.14.0. uses the Kellogg process, where the ammonia converter operates at a temperature of 437.60 °C and a pressure of 141.9 bar. From the environmental aspect, as much as 68.34 tons/h of ammonia produced produces CO_2 71.36 tons/h, which is a total emission of 1.06 tons CO_2/ tons NH_3. In this study, CO_2 delivery with a pipe length of 85 km (ID:539.8mm; OD: 558.7mm) was simulated using default parameters in Aspen Hysys V.14.0. In economic calculations from APEA (Aspen Process Economic Analyzer), the manufacture of blue ammonia designed in this study is very large, with a TAC (Total Annual Cost) of \$$82.25x10^6$/year and an LCOA (Levelized Cost of Ammonia) of \$$93.28x10^8$/ tons NH_3. This study demonstrates the integration of CCUS technology into ammonia production, resulting in a reduction of CO_2 emissions by 1.06 tons CO_2 per ton of ammonia produced. The proposed system provides a practical approach for improving the environmental sustainability of industrial chemical processes.

Keywords:
Blue Ammonia;
Carbon Emission;
Carbon Utilization;
Enhanced Oil Recovery;
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INTRODUCTION

The concentration of carbon dioxide (CO_2) in the atmosphere, which is the cause of greenhouse gas (GHG) emissions, has reached up to 410 ppm in 2019 and will continue to increase to 450 ppm in 2035 [1][2]. Several efforts have been made in Indonesia, such as utilizing exhaust gas in HRSG (Heat Recovery Steam Generator) boilers [3] and evaluating solar thermal energy in industry, especially in the East Java area [4]. Not only that, in dealing with GHG emissions, researchers in Indonesia have developed Carbon Capture and Storage (CCS) technology in various ways [5][6]. CCS technology consists of several process stages: (i) capturing CO_2 from the exhaust gas, (ii) separating CO_2, and (iii) storing it permanently in geological storage, which needs to be evaluated for economic value before a detailed engineering design is carried out [7].

The development of CCUS (Carbon Capture, Utilization, and Storage) technology is one of the options for controlling problems that arise in CCS planning in Indonesia, considering the distance of sources and storage, and the availability of operating time [8]. CCUS system planning needs to consider several factors to obtain a feasible system design that reduces CO_2 emissions and is economically competitive. The success of CCUS integration depends on whether the CO_2 utilized can provide sufficient revenue to compensate for the cost of CO_2 storage. This is because CO_2 utilization provides more positive economic value [9][10].

One of the CCUS technologies that is starting to be developed in Indonesia is enhanced oil recovery (EOR). EOR technology can reduce costs in the CCS network and reduce CO_2 emissions, making it a promising indicator for targeting CCSU [11]. In CO_2 capture, several technologies are often used by researchers, such as chemical adsorption, cryogenic distillation, membranes, and even CFZ (Controlled Freeze Zone) [12, 13, 14, 15]. Absorption technology has been widely applied in the industry due to its higher efficiency and lower pre-treatment requirements compared to other CO_2 separation processes [16, 17, 18]. Technology screening is carried out to identify feasible CCUS technology. As a result, several technologies were selected as candidates for further development under capture, transport, storage, and utilization [19, 20, 21].

One of the industries that produces quite significant CO_2 emissions is the ammonia industry [22]. The ammonia industry is one of the chemical industries that is currently experiencing global growth [23]. Most of the ammonia industry uses natural gas as a raw material for making ammonia through the steam reforming process [24]. The ammonia manufacturing process involves several steps, including desulfurization, steam reforming, a shift converter, CO_2 removal, methanation, and refrigeration units. Ammonia production is one of the most important and widely used chemical industries in the world, especially in the manufacture of fertilizers that support the agricultural sector [25]. However, the conventional ammonia production process through the Haber-Bosch process is known as one of the sources of carbon dioxide emissions, where nitrogen from the air is reacted with hydrogen to produce ammonia [26]. Hydrogen from the Steam Methane Reforming (SMR) process produces hydrogen and CO_2 as by-products [27].

CO_2 emissions generated from the SMR process will be separated using chemical absorption technology [28][29]. The chemical absorption technology proposed in this study is utilized to capture carbon emissions from the production of ammonia and natural gas with high CO_2 content. Furthermore, the CO_2 that has been successfully separated will be injected into the well and push the remaining oil to the surface, while the CO_2 gas will be trapped in the well rock. The process of reducing CO_2 emissions from the ammonia manufacturing process makes the ammonia industry known as blue ammonia [30].

The production of blue ammonia proposed in this study will be established in East Java, Indonesia, due to the availability of raw materials and geological storage locations for CO_2 storage. Natural gas, which is the raw material for ammonia, will be taken from gas wells in Bojonegoro, which contain 35% CO_2 [13]. The high CO_2 content in natural gas has led researchers to propose that CO_2 separation be carried out as a pretreatment before entering the main process in the production of blue ammonia. CO_2 emissions from the ammonia production process and impurities from this natural gas will be stored in geological storage in Sukowati, East Java. The Sukowati area has an abandoned well that can be used as geological storage [31].

The increasing production of ammonia globally has led researchers to propose the creation of blue ammonia, which is lower in emissions and more economical. This supports the government's program to develop innovations based on effective and efficient carbon capture and utilization technology to address carbon offsets for the industry in Indonesia. It is also hoped that the results of this study will serve as a parameter for comprehensively assessing the performance of the CCUS system, considering both CO2 capture technology and its utilization for EOR as a carbon offset mechanism for the chemical industry in Indonesia.

METHOD

Process Description of Blue Ammonia Production

The initial stage of planning and designing carbon emission capture in blue ammonia production involves defining the problem being investigated. The carbon emission cycle in this study consists of capturing CO_2 from the separation of natural gas and the output of the SMR and shift converter processes. In this study, the production of blue ammonia will be simulated using Aspen Hysys V.14.0. Based on research by Anugraha et al. [13], The flow rate used in this study was 40 tonsne/h (1,484 kgmole/h) or 10% of the amount of natural gas produced in the Bojonegoro gas well (456.36 tons/h or 340 MMSCFD). In contrast, the composition and operating conditions of the natural gas used as feed are shown in Table 1.

Table 1. Operating Conditions and Composition in Feed [13]

Component	Values
CH_4	60.14
C_2H_6	2.29
C_3H_8	0.68
i-C_4H_{10}	0.21
n-C_4H_{10}	0.19
i-C_5H_{12}	0.08
n-C_5H_{12}	0.06
n-C_6H_{14}	0.09
n-C_7H_{16}	0.06
n-C_8H_{18}	0.05
N_2	0.34
H_2S	0.72
CO_2	35.09
H_2O	0
O_2	0
Total	100
Pressure (bar)	41.71
Temperature (°C)	100.28

In this study, natural gas as a raw material for blue ammonia production is separated from H_2S and CO_2 using MDEA, which is gaining popularity due to lower energy requirements for solvent regeneration [30][32]. The desulfurization process of acid compounds is a process of removing impurities, because it causes corrosion and damage to the equipment [33][34]. After the desulfurization process, natural gas is reacted using steam in the SMR to produce hydrogen and carbon monoxide. Furthermore, carbon monoxide (CO) will react with the remaining steam from the SMR to be converted into hydrogen in the shift converter process. This process will produce CO_2, which will be separated in CO_2 removal using the same technology as the desulfurization process.

The CO_2 gas that is successfully separated will be used as a by-product, such as EOR. The remaining CO_2 and CO that are not separated will be converted into methane in the methanation process which the flow diagram shown in Figure 1.

Figure 1 shows that the hydrogen and nitrogen flow coming out of the methanation will be reacted in the ammonia converter reactor using the Kellogg process. The reactions that occur during the ammonia production process have been listed in the research of [27]. In this proposal, the ammonia produced is blue ammonia because the proposed process considers emissions to be reduced before being discharged into the environment. The CO_2 content formed in this process will be used to increase oil production in EOR technology, so it needs to be purified to reach 95%. The EOR process is one of the options in CCUS technology, and this proposal will inject CO_2 into the oil wells in East Java, Indonesia.

Data Collection and Process Simulation

The entire process of making blue ammonia to deliver to the oil well for the EOR process is simulated using Aspen Hysys V.14.0. Producing blue ammonia using Aspen Hysys will make it easier to get results because the Aspen Hysys database is extensive and can be used for several processes. This research uses Peng-Robinson and Acid Gas: Chemical Solvent for the fluid package in Aspen Hysys. The acid gas was used for desulfurization and CO_2 removal, and the absorber and stripper equipment were used. For other equipment, use Peng-Robinson as a fluid package because it completes calculations with high reliability and accuracy with single, binary, or tertiary phases. Meanwhile, Acid gas, a Chemical Solvent, is chosen because it is suitable for MDEA (methyl di-ethanolamine), which is a solvent for capturing acid gas from natural gas [27]. Some of the data used in this study will follow the default from the Aspen Hysys database. Other variables, such as operating condition data, are shown in Table 2.

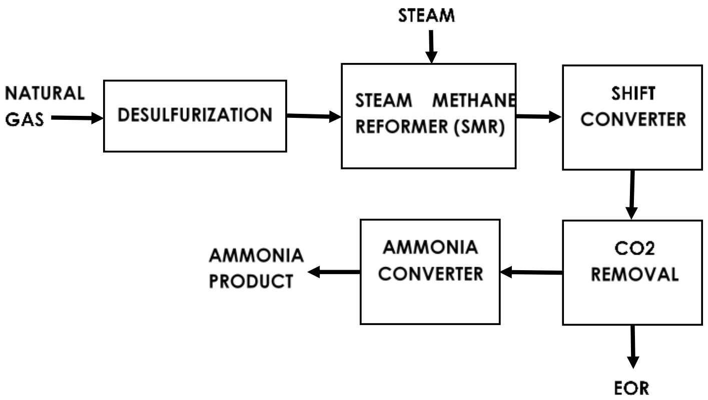

Figure 1. Flow diagram of Blue Ammonia Production

Table 2. Operating Condition in Equipment

Types of equipment	Temp. (°C)	P (bar)	Add. Parameter
Main Equipment			
Absorber 1 (AB-101)	T1: 43.05; Tn: 51.25	P1: 53; Pn: 55	25 tray
Stripper 1 (D-101)	Tc: -83.76; Tr: 8.84	Pc: 35.10; Pr: 33.01	10 stage
Primary Reformer (R-101)	650	50.35	-
Secondary Reformer (R-102)	800	34	-
High-Temperature Shift Converter (R-103)	403	34	-
Low-Temperature Shift Converter (R-104)	218.4	33.88	-
Absorber 1 (AB-102)	T1: 50.11; Tn: 74.18	P1: 36.6; Pn: 35.91	25 tray
Stripper 1 (D-102)	Tc: 30.59; Tr: 257.2	Pc: 36.91; Pr: 35.83	10 stage
Methanation (R-105)	560.6	34.67	-
Ammonia Converter (R-106)	437.6	141.9	-
Piping CO_2 Transport (estimated 85 km)	37.93	36.75	ID:539.8mm; OD: 558.7mm;
Utility Equipment			
Heater (H-101)	567	53	-
Cooler (C-101)	325	34	
Cooler (C-102)	193	33.88	-
Cooler (C-103)	189	32.98	-
Heater (H-102)	300	34.67	-
Heat Exchanger (E-101)	20	34.67	-
Compressor (K-101)	252	141.9	-
Heater (H-103)	350	141.9	-

Economic Evaluation

This research will analyze the cost of producing blue ammonia using the Aspen Process Economic Analyzer (APEA). APEA maximizes project profitability by comparing the cash flow and operating costs of multiple design options during conceptual design. APEA estimates project capital costs and asset lifecycle economics from conceptual definition through detailed engineering [35]. It has cost estimating, scheduling, and benchmarking capabilities to help users successfully manage CAPEX (Capital Expenditure) and OPEX (Operational Expenditure) [36]. This research uses CAPEX and OPEX data from APEA to calculate the TAC (Total Annual Cost) of the blue ammonia production process. The TAC, which is shown in (1), and LCOA (Levelized Cost of Ammonia) in (2), are calculated using the Luyben [37].

$$\boldsymbol{TAC} = \boldsymbol{TOC}\ (\$/\boldsymbol{year}) + \frac{\boldsymbol{TCC}\ (\$)}{\boldsymbol{PB}\ (\boldsymbol{year})} \quad (1)$$

where TAC is the total annual cost ($/yr), TOC is the total operating cost ($/yr), TCC is the total capital cost ($), and PB represents the payback period (yr).

$$\boldsymbol{LCOA} = \frac{\boldsymbol{Total\ Operating\ Cost}\ (\frac{\$}{\boldsymbol{year}})}{\boldsymbol{Total\ Product\ Capacity}\ (\boldsymbol{ton})} \quad (2)$$

where the LCOA value is calculated by dividing the total operational cost (TOC) by the amount produced per unit.

RESULTS AND DISCUSSION

Production of blue ammonia

As one of the industries contributing to carbon emissions in Indonesia, researchers are evaluating more environmentally friendly ammonia production. This is in line with emission targeting in Indonesia, where PT. Pupuk Indonesia, as an ammonia fertilizer producer, has formulated a strategic roadmap with three stages of development [38]. One of the studies under PT. Pupuk Indonesia's strategic roadmap is where researchers assess the techno-economic and environmental aspects of ammonia production [30]. Based on previous research, researchers propose an evaluation of blue ammonia production with the CCUS concept, where the carbon emissions produced will be utilized to increase oil recovery in East Java, Indonesia. Ammonia produced by combining traditional production with carbon capture and utilization or carbon capture and storage of up to 90% of carbon emissions from conventional ammonia production is called blue ammonia [30].

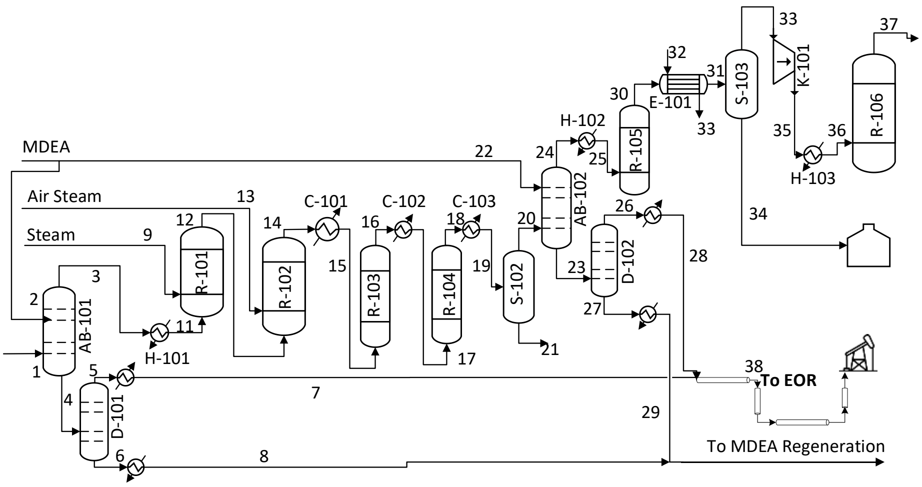

Figure 2. Process of Blue Ammonia Production

In this study, the blue ammonia production process simulated with Aspen Hysys V.14.0 is shown in Figure 2. Natural gas taken from a gas well in Bojonegoro with a CO_2 content of 35% is one of the problems that must be considered in manufacturing ammonia. The CO_2 removal process, which is generally carried out after the SMR and Shift Converter processes, needs to be added as a feed gas pre-treatment to remove acid gas. The CO_2 removal technology in this study uses chemical absorption technology. Acid gas removal at the pre-treatment stage of natural gas uses MDEA as a solvent with a concentration of 80%, as much as 250 tons/h. Chemical absorption technology using amine solvents is able to separate carbon to a CO_2 concentration of around 95% from 35% in the feed gas [14]. Acid gas that has been separated from hydrocarbon compounds will be stored and combined with the CO_2 removal results after the SMR and Shift Converter processes (Stream 7 and 28).

Air and steam reacting with sweet gas or hydrocarbons in the reformer (R-101 and R-102) will produce hydrogen and methane (stream 14). If the process air flow changes, the reformer temperature must be considered. The increase in air will increase the temperature, and to maintain operating conditions, combustion in the primary reformer must be reduced. If conditions are at optimum and changes are needed in the feed gas flow, a comparable change must be made in the air flow to maintain the N_2 and H_2 ratio. In addition to hydrogen and methane, CO and H_2O gases are converted in shift converters (R-103 and R-104) at a temperature of 200-400^{0}C (33-34 bar) to form H_2 and CO_2 emissions in stream 18. CO_2 gas needs to be removed before going to the ammonia converter process. CO and CO_2 emissions are toxic to the catalyst in the ammonia converter, so both of these substances must be removed in the CO_2 removal unit. The CO_2 removal process in this study uses the same technology as the feed gas pre-treatment at the beginning of the process. The difference in the CO_2 removal process using MDEA with a lower concentration than the feed gas pre-treatment process. As much as 50% MDEA, 3,000 tons/h is used to separate CO_2 to reach 95.25% mole.

After CO_2 gas is removed from the main stream containing N_2 and H_2 (stream 25), which still contains CO, it will be converted to CH_4 in the methanation process (R-105). The methanation reactor operates at a temperature of 560.60 °C and 34.67 bar, converting CO to CH_4 up to 100%. Not only CO but also CO_2 gas in small amounts will be converted to CH_4 in the methanation reactor using a nickel catalyst [39]. Furthermore, stream 30 is cooled to 2000 °C using cooling water of 55,000 kgmole/h in the heat exchanger (E-101) before separating N_2 and H_2 in stream 33 with methane compounds in stream 34. The ratio of H_2 and N_2 needs to be taken into consideration. If the ratio is not proper, the ammonia converter will be affected. The manufacture of blue ammonia in this study used the Kellogg process, using air and natural gas operating at a temperature of 400-600 ^{0}C and a pressure of 100-200 bar [40]. Stream 33 enters the ammonia converter reactor (R-106), operating at a temperature of 437.6 °C and 141.9 bar. The ammonia product produced in this study was 6,229.20 kgmole/h (68.34 tons/h or 0.0086 tons/year) in stream 37, which still contains nitrogen, so it needs to be purified to 99.84% of the specifications shown in Table 3.

Table 3. Specifications of Blue Ammonia Product

Component	Ammonia Product (Stream 37)	CO_2 Product (Stream 38)
CH_4	0	0.29
N_2	0.03	0.50
CO_2	0	95.25
H_2S	0	0.68
H_2O	0	0.18
H_2	0.13	3.10
NH_3	99.84	0
Total (%mole)	100	100
Flowrate (kgmole/h)	6,239.18	2,298.43
Mass flow (kg/h)	68,453.38	68,101.61
Temperature (⁰C)	437.6	35
Pressure (bar)	141.9	36

From Table 3, the amount of CO_2 produced from the design of the blue ammonia plant is 2,189.25 kgmole/h (64.87 tons/h or 0.0082 tons/year). In the process of making blue ammonia, two types of gas emissions need to be considered. Emissions from direct carbon in the ammonia production process and indirect carbon emissions from the power plant used to manufacture blue ammonia [33][41]. Not only power plants but also indirect emissions come from the combustion of natural gas used as feed for the reformer and the combustion of natural gas fuel for the boiler to generate electricity, with the assumption of a total emission of 10% [30]. The total emissions produced from the proposed ammonia production are 3,068.18 kgmole/h (71.36 tons/ h or 0.0091 tons/ year) after adding 10% indirect emissions to the amount of CO_2 produced. The total emissions successfully utilized for EOR in Sukowati were 1.06 tons CO_2/ tons NH_3. The total emissions produced from the design of blue ammonia in this study were lower than those of [30], which is 2.73 tons CO_2/ tons NH_3 for grey ammonia and 0.28 tons CO_2/ tons NH_3. This difference still exceeds the total emissions produced in grey ammonia, where emissions are directly discharged into the atmosphere. This aligns with the objectives of the CCUS system, which can reduce total emissions from industry.

CO_2 Transport

In the proposed study, CO_2 is a by-product that will be utilized to increase oil recovery in Sukowati, East Java. A reliable, economical, and safe transportation system influences the feasibility of a CCS/CCUS project. There are several transportation facilities to distribute CO_2, ranging from pipelines, tanker trucks, train tankers, and tankers, depending on the volume [8, 31, 42]. In addition to the volume of CO_2 gas to be shipped, the distance between the CO_2 production source and the utilization sink must also be considered when choosing the gas shipping process. The shipping of more than 8 billion tons of CO_2 will use pipes in 2050. This is in line with the research of [42], which evaluated the delivery of CO_2 using pipes with varying source-to-sink distances.

The ammonia production proposed in this study, CO_2 gas that was successfully purified up to 95.25% in the CO_2 removal and desulfurization process, as much as 2,189.25 kgmole/h (Table 3) was sent to the oil well in Sukowati using a pipe. The distance between the ammonia factory and the oil well is approximately 85 km. According to [8], the most effective CO_2 transportation design is in the same area because the distance between the source and sink is not too far. In this study, CO_2 delivery with a pipe length of 85 km was simulated using default parameters in Aspen Hysys V.14.0. Before being sent to the oil well, the CO_2 gas that comes out of the CO_2 removal and desulfurization process is converted into supercritical or dense form by being pressurized up to 150 bar. The process of sending CO_2 through a pipe requires several additional tools, such as a compressor and a booster [31]. The pipeline network has the advantage of systematically delivering CO_2, which consists of pipe design, process, specifications, risks, and safety.

The delivery of CO_2 to oil wells in Sukowati for the EOR process in this study was not simulated in Aspen Hysys V.14.0. However, in the CO_2-EOR injection process, it depends on the pressure and volume of the oil wells, which are still considered when analyzing the CCUS network [42]. The reservoir pressure and volume change due to fluid production from the production wells injected with CO_2. The injected CO_2 causes an additional load on the surrounding production wells. In addition, analyzing and evaluating oil wells to predict the connection between each well in one area is quite important in the EOR process. Deficiencies in the CO_2-EOR injection process will increase production, but this process also increases the corrosion rate in the pipe. So, it is necessary to get a clearer understanding of the well conditions and to design the life of the well in Sukowati based on technical and economic feasibility [43].

Economic Analysis

The economic analysis of this study is based on the results of the blue ammonia plant design simulation in Aspen Hysys V.14.0. After the blue ammonia design was simulated, the researcher activated APEA in Aspen Hysys and calculated the economic aspects of the total capital cost to the total installed cost as shown in Table 4.

Total capital cost includes equipment cost, which has been calculated in total installed cost, including converter unit, reformer unit, removal unit, and indirect cost. The total operating cost comprises the total utility cost used to design the blue ammonia plant, including raw materials and utilities. The design of the blue ammonia plant, calculated using APEA, includes sending CO_2 to an oil well using a pipe. While the payback period is assumed to be 10 years[15]. So, the total annual cost is obtained as much as $82,253,230/year. The TAC value in this study is quite large because TOC is relatively large. This can be caused by the high utilities used in designing blue ammonia plants. The design of the proposed blue ammonia plant uses many utilities, such as water, air, steam, propane, and electricity, as shown in Table 5.

In addition to calculating total emissions, researchers also calculated the LCOA based on the blue ammonia plant design. The LCOA (Levelized Cost of Ammonia) of this proposal is $93.28 x 10^8 / tons NH_3 and $97.83 x 10^8 / tons CO_2. This study has a larger LCOA than that conducted by [30], which is $ 390/ tons NH_3 for blue ammonia and $ 37/ tons CO_2. The LCOA value for blue ammonia production has considered the costs of CO_2 capture, transport, and storage. Similar to the findings in the study by Asgharian *et al.* [44], the cost of capturing CO_2 in 2022 was approximately $ 45.1 per ton, which is lower than the typical expenses associated with conventional amine-based capture technologies.

Table 4. Economic aspect of this study

Parameter	Value
Total Capital Cost ($)	20,287,300
Total Operating Cost ($/year)	80,224,500
Total Utilities Cost ($/year)	72,076,800
Equipment Cost ($)	10,338,600
Total Installed Cost ($)	17,790,900
Payback Period (year)	10
Total Annual Cost ($/year)	82,253,230

Table 5. Utility Requirement of this study

Equipment	Fluid	Value
Electricity		13,937,507 kW
Cooling Water	Water	1,241,091 BTU/h
Air Steam	Air	22,328,430 BTU/h
Heater	Steam	2,325,264,475 BTU/h
Cooler	Propane	58,795,230 BTU/h

Although quite large, the design of this blue ammonia plant can be considered by the industry in supporting emission reduction using the CCUS system.

CONCLUSION

The design of the blue ammonia plant considers technical, economic, and environmental considerations simulated using Aspen Hysys V.14.0. Technically, the manufacture of blue ammonia in this study uses the Kellogg process, commonly used in the ammonia industry. By using CCUS technology, this study contributes to reducing carbon emissions and providing a more environmentally friendly ammonia supply in East Java, Indonesia. On the other hand, environmental evaluation is seen from the total emissions formed. As much as 6,229.20 kgmole/h (68.34 tons/h or 0.0086 tons/year) of ammonia produced with a purity of 99.84% produces CO_2 3,068.18 kgmole/h (71.36 tons/h or 0.0091 tons/year), which are injected into oil wells in Sukowati with total emissions of 1.06 tons CO_2/ tons NH_3. In this study, CO_2 with a purity of 95.25% delivery with a pipe length of 85 km was simulated using default parameters in Aspen Hysys V.14.0. However, in the CO_2-EOR injection process, it depends on the pressure and volume of the oil wells, which are still taken into account in analyzing the CCUS network. The reservoir pressure and volume change due to fluid production from the production wells that are injected with CO_2. In economic calculations, the manufacture of blue ammonia designed in this study is considerable, with TAC of $82,253,230/year and LCOA of 93.28 x 10^8 $ / tons NH_3 or 97.83 x 10^8 $ / tons CO_2. Although the TAC and LCOA values are quite large, the manufacture of blue ammonia in this study is expected to be considered as an innovation to calculate carbon offsets as an effort to reduce industrial emissions.

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