Project Report on

Techno-economic analysis of cryogenic CO_2 capture process in the context of Nepal and its applications

Submitted by: Bishwash Paneru

Affiliation: Department of Applied Sciences and Chemical Engineering, Pulchowk Campus, Institute of Engineering, Tribhuvan University, Lalitpur, Nepal

Project Funded by: United Engineering Foundation (UEF)

Submitted to: Sustainable Energy Corp (SEC), American Institute of Chemical Engineers (AIChE)

Abstract:

This project analyzes the proposed models for capturing CO_2 in the desired liquid phase which can be a major step in reducing the greenhouse effect caused by CO_2 emissions. The discussed models in this report demonstrate high efficiency in capturing over 99% of CO_2 from raw and flue gases produced in various industries. The analysis of cryogenic capture of CO_2 from flue gas produced by the Sarbottam Cement Industry of Nepal is done. The cost of setting up the plant, however, is noted to be very high. Still, high efficiency is achieved for the cryogenic CO_2 capture process, which shows its applicability in practical life if cost reduction methods are able to be applied. This research project also includes graphs and diagrams illustrating the composition of products, mass and energy balance at equipment and stream used, cost analysis, sensitivity analysis, and the variation of NPV (Net Present Value), and ROI (Return of Investment) with profit and time. The captured liquid CO_2 can be utilized for different applications like the formation of methanol, methane, and urea, and the cryogenic process can be used in processes like enhanced oil recovery and the Rectisol Wash Process for removing the H_2S and CO_2 from sour syngas. The results highlight the effectiveness of the proposed system in capturing CO_2 and the potential for generating very high income through the production of methanol and urea and for reducing CO_2 gas emissions and the problem of climate change.

Key points:

- CO_2 is causing greenhouse gas effects on the environment that can be reduced using the cryogenic capture.
- The proposed model shows high efficiency in capturing over 99% of CO_2 from raw gases.
- The cost of setting up the plant is noted to be very high.
- The disadvantage is the high cost, and the very high efficiency of this process is the main advantage that makes the investments in developing such projects worthy of achieving good returns on investment.
- The liquid form of CO_2 generated through the proposed system has the potential to generate a high income.
- Graphs and diagrams illustrate the composition of products and the variation of NPV with profit and time.
- The results demonstrate the very high effectiveness of the proposed models in capturing CO_2 in the desired liquid phase.
- CO_2 capture using cooling and compressing at cryogenic conditions is also applicable to enhancing process efficiency for processes like enhanced oil recovery and the Rectisol wash process for the removal of H_2S and CO_2.
- Cost reduction methods, like the utilization of the Organic Rankine Cycle (ORC), can be applied to convert the generated heat from coolers used in the process operation to regenerate electricity.
- Nepal can generate a large quantity of urea using hydrogen from water, nitrogen from air, and CO_2 produced using cryogenic CO_2.
- The cryogenic capture process can help reduce carbon emissions and hence global warming for which cost-reduction steps are necessary to be implemented.

COPYRIGHT

Bishwash Paneru

Project leader

e-mail: 076bch015.bishwash@pcampus.edu.np

Department of Applied Sciences and Chemical Engineering

Pulchowk Campus

Lalitpur

Nepal

TRIBHUVAN UNIVERSITY

INSTITUTE OF ENGINEERING, PULCHOWK CAMPUS

DEPARTMENT OF APPLIED SCIENCES AND CHEMICAL ENGINEERING

The undersigned certify that they have read and recommended the Sustainability Energy Corps (SEC) of AICHE (American Institute of Chemical Engineers) and UEF (United Engineering Foundation) for acceptance, a project report entitled "TECHNO-ECONOMIC ANALYSIS OF CRYOGENIC CO_2 CAPTURE PROCESS IN THE CONTEXT OF NEPAL AND ITS APPLICATIONS" submitted by Bishwash Paneru from Department of Applied Sciences and Chemical Engineering of Institute of Engineering, Pulchowk Campus and his team members Biplov Paneru and Anup Paudel in order to have their contribution in the UEF Funded climate solutions project.

Advisor, Asst. Prof. Dr. Ziaul Haque Ansari

Department of Applied Sciences and Chemical
Engineering, Pulchowk Campus, I.O.E, Tribhuvan
University, Lalitpur Nepal

Advisor, Prof. Dr. Khem Narayan Poudyal

Department of Applied Sciences and Chemical
Engineering, Pulchowk Campus, I.O.E, Tribhuvan
University, Lalitpur Nepal

Advisor, Prof. Dr. Hem Raj Pant

Head of Department, Department of Applied Sciences and
Chemical Engineering, Pulchowk Campus, I.O.E,
Tribhuvan University, Lalitpur Nepal

External Supervisor, Dr. Ramhari Poudyal

Visiting Professor, Purwanchal University, HIST
Engineering College, Lalitpur Nepal

Date: 11/09/2023

ACKNOWLEDGEMENT

First of all, I would like to express my deepest gratitude to the Sustainable Energy Corp (SEC) of AIChE (American Institute of Chemical Engineers) and UEF (United Engineering Foundation) for accepting me and my team members in the UEF-funded grant program for climate change solutions project to have our contributions in solving global climate change problem and UEF for funding this project. Also, I am thankful to Wendy Young (Senior Director of the Institute for Learning & Innovation) and Jeffrey Perez (Education Specialist) of the AIChE for providing us the guidance during the overall project report creation and submission phase. I am also thankful to DWSIM's development team for providing the software for free for learners and to those contributors of DWSIM's simulation models as examples for learners accessed from the website of **Completed Flowsheets | DWSIM (fossee.in)** who have been addressed properly in this report.

I am thankful to my team members Biplov Paneru from the Department of Electronics, Communication, and Information Engineering, Nepal Engineering College, Pokhara University, and Anup Paudel, a recent Mechanical Engineering graduate from IOE, Pulchowk Campus, Tribhuvan University, Nepal for their over help during the research work and creation and finalization of this report. I am also thankful to Prof. Dr. Hem Raj Pant, Asst. Prof. Dr. Ziaul Haque Ansari and Prof. Dr. Khem Narayan Poudyal from IOE, Pulchowk Campus, Tribhuvan University, Lalitpur, Nepal, and Dr. Ramhari Poudyal from Hist Engineering College, Purwanchal University, Lalitpur, Nepal for providing their valuable advice in preparing this research project's report.

Finally, I would also like to extend thanks to all my colleagues and seniors who helped me and my team with their valuable suggestions.

Bishwash Paneru

Department of Applied Sciences and Chemical Engineering

Tribhuvan University

Lalitpur

Nepal

Table of Contents

List of figures:

List of tables:

Some abbreviations:

1. IEA: International Energy Agency
2. CAPEX: Capital Expenditure
3. DWSIM: Dynamic Workbench for Simulation
4. USD: United States Dollar
5. GHG: Green House Gases
6. OECD: Organization for Economic Co-operation and Development
7. OPEX: Operational Expenditure
8. CO_2: Carbon Dioxide
9. AMC: Accelerated Mineral Carbonation
10. PR: Peng-Robinson
11. HP: Horsepower
12. MBR: Mass Balance Rate
13. EBR: Energy Balance Rate
14. LCCA: Levelized Cost of CO_2 Abatement
15. NPV: Net Present Value
16. ROI: Return of Investment
17. MBR: Mass Balance Ratio
18. EBR: Energy Balance Ratio
19. ABS: Advanced Business Solutions
20. CAPE-OPEN: Computer-Aided Process Engineering Open
21. SEP: Separator
22. CL: Cooler
23. SC: Shortcut Column
24. COMP: Compressor
25. PFR: Plug-Flow Reactor
26. HE: Heat Exchanger
27. MIX: Stream Mixer

28. VALV: Valve
29. SPLT: Stream Splitter
30. PM: Particulate Matter
31. SDGs: Sustainable Development Goals
32. SNCR: Selective non-catalytic reduction
33. SCR: Selective catalytic reduction
34. REDD: Reduced emissions from deforestation and degradation
35. ORC: Organic Rankine Cycle
36. PFR: Plug Flow Reactor
37. EOR: Enhanced Oil Recovery
38. EEF: Enhanced efficiency fertilizer

Equipment and some Units used:

- MBR (Mass Balance Rate)
- EBR (Energy Balance Rate)
- CAPE-OPEN Unit Operation
- Stream Splitter
- Heat Exchanger
- Cooler

Stream Units:

- Mass Flow (kg/h)
- Temperature (◦C)
- Pressure (bar)
- Energy Flow (kW)

Energy Units:

- kW (kilowatt)
- kJ/mole (kilojoule/mole)
- HP (horsepower)

Cost Units:

- United States Currency (Dollars/$)

Other Units:

- Efficiency (%)

1. Introduction

Carbon dioxide (CO_2) is a primary threat to the environment today. Most of the high- and upper-middle-income countries account for a much bigger share of emissions despite being home to just under half of the total population of the world; they emit more than 80% of the world's CO_2, while most of the lower-middle- and low-income countries emit a lower amount, less than 20% [1]. CO_2 is generated through various sources such as industrial plants, plastic combustion, refineries, vehicles, combustion of coal and natural gases, etc., and these are the major sources of the green greenhouse effect and global warming that have been a major concern to be addressed and solved today.

The International Energy Agency (IEA) publishes a detailed analysis of CO_2 emissions in its reports. According to the report on Global Energy Review 2021, despite the decline in 2020, global energy-related CO_2 emissions remained at 31.5 Gt in 2020, which contributed to CO_2 reaching its highest-ever average annual concentration in the atmosphere of 412.5 parts per million in 2020—around 50% higher than when the industrial revolution began [2]. Their report on CO_2 emissions in 2022 states that global energy-related CO_2 emissions increased by 0.9%, or 321 metric tons, in 2022, reaching a new high of over 36.8 metric tons [3].

The primary sources of greenhouse gas emissions are activities being performed by humans, which include fossil fuel combustion for electricity, heat, and transportation, as well as industrial processes and land-use changes [4][5]. The largest source of greenhouse gas emissions from human activities in the United States is from burning fossil fuels for electricity, heat, and transportation [4]. The transportation sector creates the largest share of greenhouse gas emissions, followed by electric power and industry [4]. Burning coal, natural gas, and oil for electricity and heat is the major contributing source of global greenhouse gas emissions **Error! Reference source not found.**.

Some of the major effects of CO_2 emission on the environment are as follows:

Global warming: Carbon dioxide and other greenhouse gases cause heat trapping in the atmosphere, leading to a rise in global temperatures. This heat trapping can have an effect on the whole ecosystem of the planet.

Ocean acidification: When carbon dioxide dissolves in seawater, it forms carbonic acid, which can make the water more acidic and cause a negative impact on marine life, including shellfish and coral reefs. Such effects have long-term effects, like the extinction of marine species in the ocean.

Rising sea levels: As temperatures rise, glaciers and ice sheets melt, resulting in rising sea levels, which can lead to flooding and erosion of coastlines and natural calamities.

Changes in weather patterns: Climate change can cause changes in patterns of weather, including more frequent and severe heat waves, droughts, and storms. This causes natural calamities like floods, landslides, soil erosion, etc.

Impact on human health: Climate change can have a negative impact on human health, including an increased risk of respiratory problems due to air pollution, an increased risk of heat-related illnesses, and more. Diseases like skin cancer are examples of diseases caused by the thinning of the ozone layer.

Economic impact: Climate change can have a significant economic impact, including damage to infrastructure due to extreme weather events, loss of crops due to droughts or floods, and more.

CO_2 capture from flue gas in industries like the cement industry: Flue gas is the exhaust gas emitted by industrial processes that burn fossil fuels or biomass. It contains a high concentration of CO_2, which can be captured and stored to reduce greenhouse gas emissions and mitigate climate change. There are various technologies for CO_2 capture from flue gas, such as adsorption, chemical looping, membrane gas separation, or gas hydration [6]. Some of these technologies are already in operation or under development in cement plants around the world [8] [9].

CO_2 production in Nepali industry: According to a report by the World Bank, Nepal's total CO_2 emissions in 2014 were 9.5 million tons, of which 29% came from the industrial sector [10]. The main sources of industrial emissions were cement production, brick kilns, iron and steel manufacturing, and food processing [11]. Nepal has a low-carbon development strategy that aims to reduce its emissions intensity by 20% by 2030 compared to 2010 levels [11].

CO_2 storage after capturing (tanks, systems): After CO_2 is captured from industrial sources or power plants, it needs to be transported and stored in a safe and permanent way. One option is to inject the CO_2 into deep geological formations, such as depleted oil and gas reservoirs, saline aquifers, or coal seams [12]. Another option is to convert the CO_2 into mineral carbonates, such as limestone or dolomite, through chemical reactions with rocks or industrial wastes [13]. A third option is to use the CO_2 for enhanced oil recovery (EOR), which involves injecting the CO_2 into oil wells to increase the pressure and extract more oil [14].

Uses of CO_2: CO_2 has many industrial and commercial uses, such as generating chemicals and fuels, refrigerating and carbonating beverages, welding and soldering metals, enhancing plant growth in greenhouses, and fire extinguishing [15]. CO_2 can also be used as a feedstock for making synthetic materials, such as plastics, polymers, and carbon fibers [16]. Additionally, CO_2 can be used as a medium for storing and transporting renewable energy, such as hydrogen or ammonia [17].

Methanol's uses: Methanol is a simple alcohol (CH_3OH) that can be produced from various sources, such as natural gas, coal, biomass, or CO_2. Methanol is widely used as an industrial solvent and a chemical building block for making products such as formaldehyde, acetic acid, urea, and biodiesel [18]. Methanol can also be used as a fuel for vehicles, boilers, cook stoves, or fuel cells [19].

Green hydrogen, nitrogen generation, ammonia generation, CO_2 capture, and urea in Nepal are the major areas under research and discussion at present. Green hydrogen is hydrogen produced from renewable energy sources without emitting CO_2. It can be used as a clean fuel or a chemical feedstock for various applications. Nitrogen is an essential element for life and agriculture. It can be obtained from the air by using electricity or natural gas. Ammonia is a compound of nitrogen and hydrogen (NH_3) that can be used as a fertilizer, a refrigerant, or a carrier of hydrogen. CO_2 capture is the process of removing CO_2 from industrial emissions or the atmosphere. Urea is an organic compound of carbon, nitrogen, oxygen, and hydrogen (CH_4N_2O) that can be used as a fertilizer or a raw material for plastics. Nepal has the potential to produce green hydrogen from its abundant hydropower resources and use it for domestic or export purposes [20]. Nepal also has the potential to produce ammonia and urea from its natural gas reserves and use them for agriculture or industry [21]. However, Nepal faces many challenges in developing its green hydrogen and ammonia sectors, such as a lack of infrastructure, technology transfer, financing, policy support, and market access [22].

Carbon generation from plastic: Plastic is a synthetic material made from fossil fuels that contains carbon atoms. When plastic is disposed of in landfills or incinerated, it releases carbon dioxide (CO_2) into the atmosphere. Plastic waste also contributes to ocean pollution and harms marine life. According to a study by UC Santa Barbara researchers, plastics generated 1.8 billion tonnes of CO_2 emissions in 2015 – equivalent to 3.8% of global emissions [23].

CO_2 generation from plastic in industries: Plastic production and consumption are major sources of CO_2 emissions in industries. According to the OECD report “Plastics Leakage and GHG Emissions”, plastics generated 1.8 billion metric tons of CO_2 emissions in 2019—3.4% of global emissions—with 90% of these emissions coming from their production and conversion from fossil fuels [24]. By 2060, emissions from the plastics lifecycle are set to more than double, reaching 4.3 billion metric tons of CO_2 emissions [24].

CO_2 generation by plastic pyrolysis: Plastic pyrolysis is the process of decomposing plastic waste by heating it in the absence of oxygen. It can produce useful products such as oils, gases, waxes, and carbon. However, plastic pyrolysis also generates CO_2 emissions, depending on the type and composition of the plastic and the pyrolysis conditions. According to a study by Springer researchers, plastic pyrolysis can generate between 0.1 and 0.8 kg of CO_2 per kg of plastic waste [25]. However, some of these emissions can be diminished by using the pyrolysis products as fuels or feedstocks for other processes [25].

There is a need for technology that can utilize syngas and flue gas to form CO_2 in liquid or solid form as desired with high efficiency of capture. For such purposes, CO_2 capture by cryogenic cooling and compression can be a major breakthrough, as it has high efficiency in capturing CO_2 with the simultaneous conversion of CO_2 from flue, raw, or syngas to liquid or gaseous form.

Figure 1: Diagram representing the applications of CO_2

2. Objectives

This research project for the study of the cryogenic CO_2 capture process has the following objectives:

1. To study the feasibility of CO_2 capture using compression, cooling and separation process.
2. To determine the most appropriate number of stages for CO_2 capture in cryogenic conditions
3. To estimate the costs required for overall plant setup and establishment.
4. To optimize process efficiency.
5. To determine the different applications of the captured CO_2.
6. To determine the parameters that affect the efficiency of the processes.

3. Limitations

The limitations of the overall study are mentioned below:

1. There is only a theoretical evaluation of the processes using software tools and numerical calculations.
2. The cost parameters may not be accurately measured as they are affected by various parameters in a practical scenario.

3. The data on flue gas composition for selected industries may vary yearly and can only be useful for a rough estimation of CO_2 capture feasibility in the industry.
4. The cost and expenses measured for the different processes are high, and no detailed discussion has been done to decrease such costs and expenses.

4. Literature review

A CO_2 capture plant has not been established until today in Nepal, despite Nepali industries, including cement industries like Hongshi Cement Industry, Sarbottam Cement Industry, etc., emitting greenhouse gases like CO_2. Several authors have mentioned CO_2 capture technology and its application in the context of Nepal.

Devkota et al., in their research [34], mentioned the utilization of a detailed design, cost estimation, and sensitivity analysis for establishing a CO_2 capture plant for usage in urea manufacturing in the context of Nepal. The authors performed a techno-economic analysis of CO_2 capture from flue gas generated by the Nepali cement industries. Through this research, it was found that the capital cost and the production cost for the plant of this scale are $10 million per year and $18 million per year. It was concluded by the research that the availability of cheap hydropower electricity (lower than $0.01/kWh) makes CO_2 capture-based urea manufacturing plants a viable alternative for Nepal.

Chaudhary et al., in their review article [26], mentioned the use of CO_2 capture technology for urea production in Nepal. The authors have reviewed: (i) the status of the SDGs (Sustainable Development Goals) of Nepal; (ii) agricultural productivity associated with industries and the supply of urea; (iii) technologies associated with urea production; (iv) the feasibility of establishing a urea plant based on raw material availability and sustainability; and (v) the opportunity for economic and technological development. The electricity generated from the Nepali hydropower by electrolysis process and CO_2 capture from the cement industry's flue gas were determined to be a strategically feasible and sustainable pathway for urea production and consequently the fulfillment of SDGs in the context of Nepal.

The study by Adhikari et al., [28] presented their findings from a questionnaire survey to know the pattern of energy consumption for cooking, water heating, and animal feeding in the outskirts of the Katmandu Valley. After the data collection, the total energy consumed for cooking and water heating purposes in the valley was calculated. The annual consumption of firewood in Ghimire Gaun was found to be about 23.5 tons (97,905 kWh), of which about 3.18 tons (13,235.04 kWh) are used for water heating purposes. The total amount of CO_2 reduction by one solar flat plate is around 195 kg/year. The re-boiler energy requirement for the CO_2 capture process model is around 4 MJ/kg CO_2. Therefore, the total amount of energy required to capture the CO_2 is around 195×4 MJ/year (780 MJ/year). Therefore, by installing one flat place, it can save 780 MJ/year of energy instead of capturing the CO_2 from gasification.

Khadka et al., **Error! Reference source not found.** mentioned the use of green forests as a tireless apparatus of oxygen production, which is the precious life gas for living beings. Forests produce timber and non-timber products. Besides, forests perform ecosystem services, provide biodiversity, and capture the CO_2 produced during the respiration process of living beings. Globally, the the estimated annual deforestation was -0.13%, and between 2000 and 2010, there was a positive change of 0.28% in Asia. Moreover, the annual forest area loss in Terai, Nepal, was 0.40% between 1991 and 2010.

According to K.C. et al. [29], more than 90% of the trees having a diameter of less than 20 cm indicate a high capacity for increasing biomass in the future. The ground tree biomass, ground sapling biomass, biomass in herbs and litter, and below-ground biomass were 126.3, 2.88, 7.54, and 27.34 tons/ha, respectively. The total carbon stock, annual carbon sequestration rate, and total CO_2 mitigation potential were 122.29, 0.45, and 1.64 tons/ha, respectively. Reduced emissions from deforestation and degradation (REDD) should be implemented to get the monetary benefit of carbon dioxide mitigation that will help the conservation of forests.

Sarkar et al. [30] mentioned the sustainable development goals (SDGs) based on selected indicators to capture the progress of SDGs among South Asian countries. The selected indicators are used to explore countries' achievements of the SDGs since their adoption in 2015 and the challenges of achieving specific SDGs. The results of the study also portray that the majority of South Asian countries spend less than 4% of their GDP on education and health, which hinders the progress of SDG indicators. Moreover, many countries are still far from environmental sustainability indicators such as CO_2 emissions per capita, air pollution, and forest coverage. Overall, though the countries have made some positive progress in particular SDGs, the majority of SDGs, including 1, 5, 8, 11, 14, and 17, remain challenges for achieving the target. Therefore, this study suggests that countries promote policies and initiatives targeting specific SDGs to achieve the SDGs by 2030.

In the study by Vineel et al. in their research [31], multipurpose plant setup is discussed using the concept of the House Process and various other techniques to achieve objectives like reducing atmospheric CO_2 to carbon and thus reducing global warming, producing hydrogen gas, producing electricity, and providing energy feedback for improved efficiency. These objectives are obtained through a six-stage process. In the first stage, atmospheric CO_2 is absorbed using an improvised version of the house process. In the second stage, CO_2 is produced by heating $NaHCO_3$, a by-product of the house process. In the 3rd stage, the reaction of the produced CO_2 with Mg occurs to get magnesium oxide and carbon. The 4th stage consists of the recovery of Mg from its oxide by using a modified house process and the consequent electrolysis of $MgCl_2$. In the 5th stage, energy produced by the exothermic reactions is used to produce steam and electrical energy by rotating a turbine. Finally, hydrogen gas is produced by the reaction of steam and magnesium.

The study [32] was done by authors to focus on waste-to-energy and especially its current status and benefits. According to the study, the primary source of GHG is landfill sites, which produce significant amounts of methane and carbon dioxide gas, and the main impact of the methane is on a global scale as a greenhouse gas. Although levels of methane in the environment are relatively low, its high "global warming potential" (21 times that of carbon dioxide) ranks it among the worst of greenhouse gases. The main cause of the uplift in atmospheric temperature is the high production of GHG (CH_4, CO_2, N_2O, etc.). GHG reduction measured in waste consists of source reduction through waste prevention, recycling, composting, waste to energy incineration, methane capture from landfills, and waste water. Specific reduction options include the use of the 3R principle, waste segregation, reduction at source, composting anaerobic digestion for biogas, sanitary landfill sites with methane capture, healthcare waste management, a proper statutory framework, public participation, private sector partnerships, tax waivers for recycling enterprises, and financial management. Regulation is essential to ban recyclable waste from landfills.

Devkota et al. [34], delivered the assessment of the ammonia production plant technically and economically and have mentioned the use of ammonia for the urea production capacity of Nepal. According to this article, CO_2 is generally captured using a liquid solvent, which is then heated to separate the gas. Finally, urea is produced by catalytically reacting CO_2 and NH_3 at high temperatures and pressures. H_2 can also be obtained from water electrolysis, and CO_2 can be captured from the exhaust of cement, steel, and power plants. Ammonia (NH_3) and carbon dioxide (CO_2) are the major raw materials for manufacturing urea. NH_3, in turn, is made by reacting nitrogen (N_2) and hydrogen (H_2). N_2 can be directly captured from the air. H_2 can also be obtained from water electrolysis, and CO_2 can be captured from the exhaust of cement, steel, and power plants. Electrolysis and carbon capture are both energy-intensive processes, which has limited this pathway of urea production. The study gives a pathway for research and development of the overall urea development plant.

There are many research articles available, and research is being conducted on methods of CO_2 capture, but the best method for CO_2 capture is not fixed since cost, efficiency, and many other related parameters affect it. Similarly, in the context of Nepal, no proper research has been conducted to determine the feasibility of CO_2 capture using cryogenic separation technology.

5. Methodology

5.1. Pretreatment

In order to capture CO_2 from flue gas or raw gas, preprocessing and treatment are necessary. Pretreatment of flue and raw gases before carbon dioxide capture is necessary to reduce the efficiency of the capture process. The common impurities include nitrogen oxides (NO_x), sulfur dioxide (SO_2), and dust particulates.

Dust and particulates can clog the capture equipment and have a huge effect on its efficiency. Such clogging reduces the efficiency of the equipment, and hence, the overall process efficiency gets affected. The dust and particulates can ultimately cause a rise in maintenance and repair costs. Dust and particulates can be removed using a variety of methods, such as electrostatic precipitators, cyclones, and bag filters.

Sulphur dioxide (SO_2) can react with the CO_2 capture solvent to generate the corrosive compounds. It can also decrease the efficiency of the overall carbon capture process. SO_2 can be removed using the different methods, such as wet scrubbing, dry scrubbing, and limestone injection.

Nitrogen oxides (NO_x) can react with the CO_2 capture solvent to generate many harmful compounds. They can also decrease the efficiency of the carbon capture process. NO_x can be removed using a variety of methods, such as C (SCR) and selective non-catalytic reduction (SNCR).

The specific pretreatment steps required will depend on the composition of the flue or raw gas and the type of CO_2 capture technology that is being used. For example, if the flue gas contains a high amount of SO_2, a wet scrubber may be essential. If a flue gas contains a high concentration of NO_x, SCR or SNCR may be required. Processes like AMC (accelerated mineral carbonation) can be used has the potential to decrease overall cost associated with CO_2 separation/compression/transportation/pore space/brine water treatment [35].

Here are some examples of pretreatment technologies used for flue and raw gas before CO_2 capture:

- **Cyclones:** Cyclones are used for the removal of large amounts of dust particles from the gas stream.
- **Electrostatic precipitators:** Electrostatic precipitators are used to remove impurities from the gas stream.
- **Bag filters:** They are used to remove very fine dust particles from the gas stream.
- **Wet scrubbers:** Wet scrubbers use a dry sorbent to remove the impurities from the gas stream.
- **Limestone injection:** It is a process that is used for the removal of SO_2 from the gas stream.
- **Selective catalytic reduction (SCR):** SCR is a process that is used to remove NOx from the gas stream using a catalyst.
- **Selective non-catalytic reduction (SNCR):** SNCR is a process that is used for the removal of NO_x from a stream using a catalyst.

The choice of pretreatment technology will depend on a number of factors, including the composition of the flue or raw gas, the type of CO_2 capture technology being used, and the desired level of purity of the captured CO_2.

Figure 2: Diagram representing CO_2's reutilization

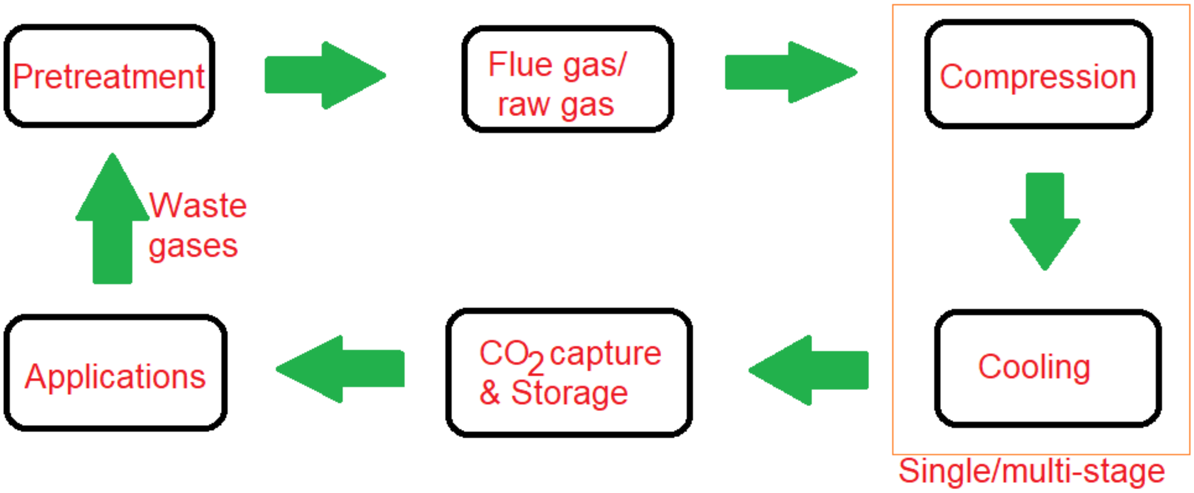


Figure 3: Overall CO_2 capture and recycle process

5.2. CO_2 Capture in the gaseous and liquid phase from raw gas (Techno-economic analysis)

The CO_2 capture process can be designed and optimized to get all necessary information about the process with special software for simulation and modeling like Aspen Plus, Aspen Hysys, Pro II, Simulink, DWSIM, etc. Since DWSIM is one of the simpler yet popular programs for process modeling and optimization, we decided to use DWSIM software for our analysis.

DWSIM is an open-source chemical process simulation software that allows users to model and simulate chemical processes using advanced thermodynamic models and unit operations. It is available for Windows, macOS, and Linux operating systems. DWSIM supports a wide range of thermodynamic models, including the Peng-Robinson, Soave-Redlich-Kwong, and UNIFAC models, among others. It also includes a comprehensive library of unit operations, such as distillation columns, heat exchangers, reactors, and more. DWSIM is designed to be user-friendly and includes a graphical user interface (GUI) that allows users to create and edit process flowsheets easily.

5.2.1. CO_2 capture in the gaseous phase

We propose a model based on compression followed by cooling and separation until CO_2 is produced in a gasified form. The major purpose of the proposed model is to determine the plant setup required to check the feasibility of complete CO_2 capture in industries. In the context of CO_2 capture, compression refers to increasing the pressure of the gas to make it easier to transport. Cooling, on the other hand, involves reducing the temperature of the gas to make it easier to store.

This process of cryogenic compression and cooling uses low temperatures to separate gases. It is used to capture CO_2 from a variety of sources, including power plant flue gas, industrial emissions, and even the atmosphere. The process works by compression which is typically done using compressors, which force the gas molecules closer together, leading to an increase in pressure. The goal is to achieve a pressure level suitable for the subsequent cooling step which involves cooling the gas stream to a very low temperature, typically below -78 °C. At this temperature, CO_2 liquefies and can be separated from the other gases in the mixture. The liquid CO_2 is then collected and can be stored or used for other purposes.

Cryogenic separation is a relatively energy-intensive process, but it is one of the most efficient ways to capture CO_2. It is also a scalable process, meaning that it can be used to capture CO_2 from large or small sources.

Many industries produce raw gases with various components that are harmful, along with CO_2. Let us take an example of a raw gas consisting of CO_2, water, methane, ethanol, methanol, nitrogen, dimethyl sulfide, and acetaldehyde. If we take an example of this raw gas consisting of the following composition as mentioned in Table 1, it is produced by industries such as the fertilizer industry, paper and pulp mills, wastewater treatment plants, natural gas production plants, etc. The proposed simulation model in Figure 4Figure 4 can be used to capture the CO_2 constituent in gaseous form.

Table 1: Feed raw gas composition

S.No	Composition	Feed flow rate (kg/s)	Percentage of component
1	Carbon dioxide	1979.5628	98.97814
2	Water	14.915229	0.74576145
3	Methane	1.4019773	0.070098865
4	Ethanol	2.2883618	0.11441809
5	Methanol	0.85479528	0.042739764
6	Nitrogen	0.36077818	0.018038909
7	Dimethyl Sulphide	0.49441553	0.024720777
8	Acetaldehyde	0.12157347	0.006078674
9	Total	1999.999931	100

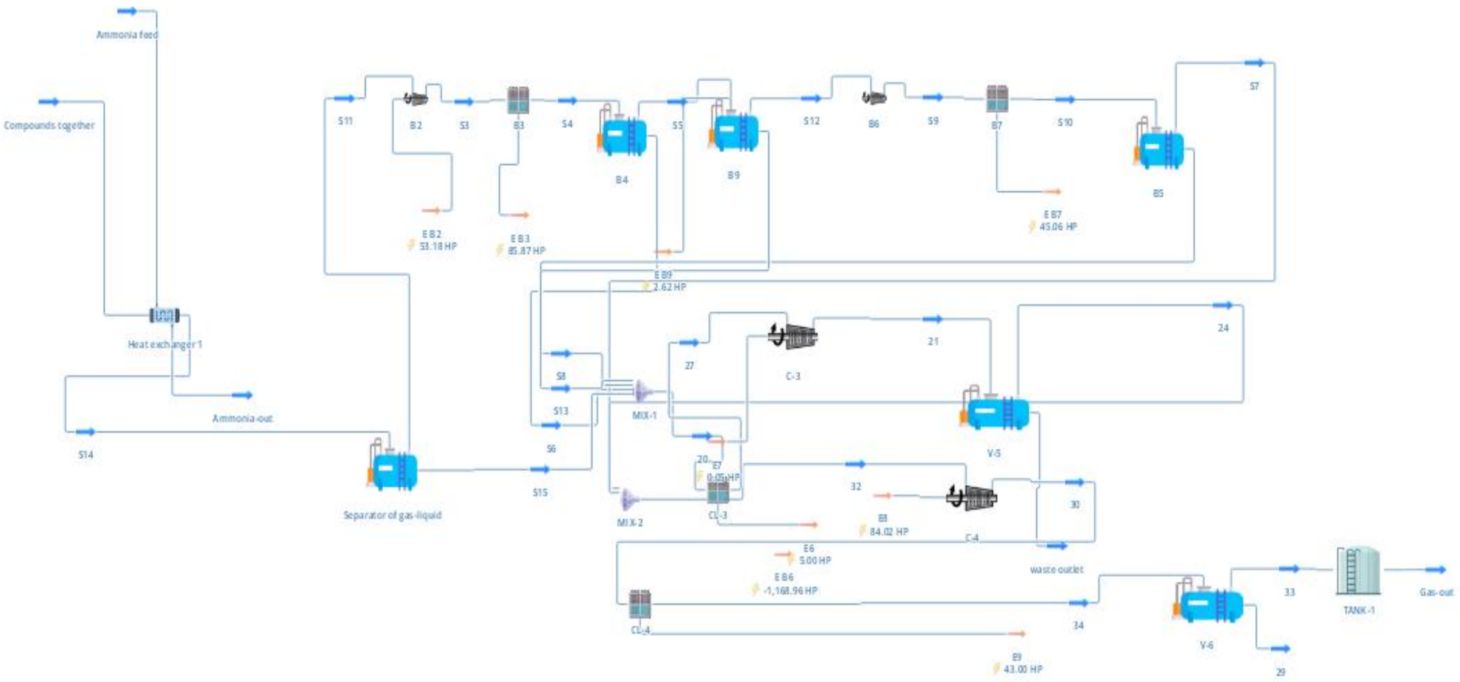


Figure 4: 99% capture of CO_2 from raw gas mixture

The entire process flow diagram for the production of liquid carbon dioxide is simulated in DWSIM (v8.5). The raw gas composition is taken from available industrial data. The Peng-Robinson (PR) equation of state is used as a thermodynamic model to incorporate variation from the ideal behavior of the raw gas feed.

A shell and tube heat exchanger is simulated with ammonia as the refrigerant and a feed rate of 900 kg/h for the raw gas cooler. Ammonia is sent on the shell side, and raw gas is sent on the tube side. The inlet conditions for the ammonia and design variables are taken from the available industrial raw gas data.

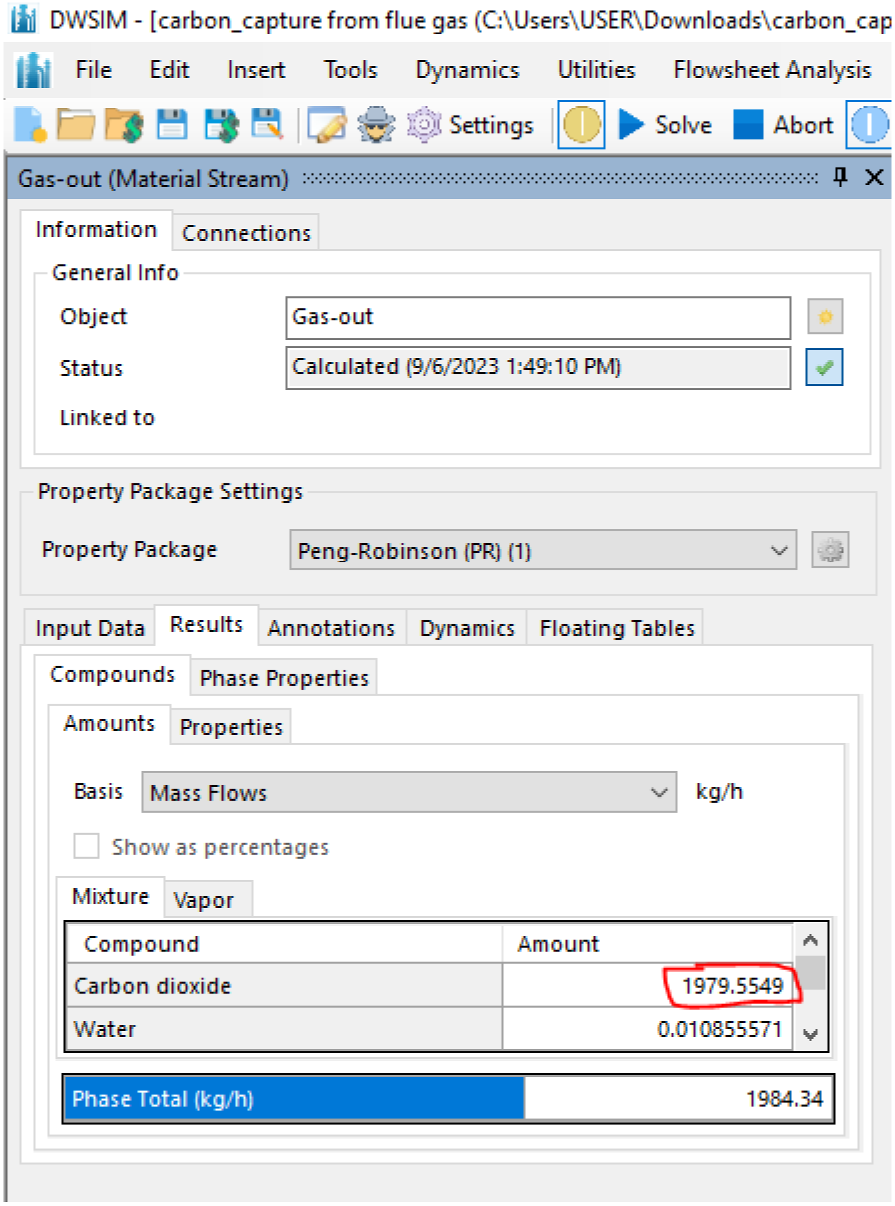
The PR (Peng-Robinson) property package was used for all components. A vacuum-liquid separator (like B4) is used after the raw gas cooler to separate the liquid in the stream before compression. Adiabatic compressors with an efficiency of 75% are used before the two flash columns. Coolers with an efficiency of 100% are used after the flash columns.

In the first flash column, water and methanol are removed from the liquid stream, while carbon dioxide is recovered with other components in the vapor stream. In the second flash column, carbon dioxide is recovered in the liquid stream along with ethanol, dimethyl sulfide, and other components.

The total flow rate of the feed stream was maintained at 2000 kg/h overall for raw gas composition, with temperature and pressure maintained at 25 $^{\circ}$C and pressure of 1 bar. Gaseous carbon dioxide is obtained with more than 99% purity in the stream (gas-out) as shown in table below.

Table 2: Product composition at gas-out stream

Composition	Product/hour
Carbon dioxide	1779.555
Water	0.010856
Methane	1.401977
Ethanol	2.887349
Methanol	0.067285
Nitrogen	0.360778
Dimethyl Sulphide	0.494409
Acetaldehyde	0.121572
Total	1784.899



Object: Gas-out

Status: Calculated (9/6/2023 1:49:10 PM)

Linked to

Property Package: Peng-Robinson (PR) (1)

Basis: Mass Flows kg/h

Compound	Amount
Carbon dioxide	1979.5549
Water	0.010855571

Phase Total (kg/h): 1984.34

Figure 5: Captured CO_2 outflow through Gas-out stream

The mass and energy balance for the individual streams and the equipment used in the overall process are as follows:

Table 3: Mass and energy balance for equipment

Equipment	Type	Energy Consumption (-) / Generation (+) (HP)	Efficiency (%)	MBR (kg/h)	EBR (HP)
C-4	Compressor	-84.0151	75	0	-9.8795E-10
CL-3	Cooler	5	100	0	-2.94554E-10
MIX-2	Stream Mixer	9.55617E-06		1.59872E-12	-9.55617E-06
C-3	Compressor	-0.0477344	75	0	9.90045E-05
V-5	Gas-Liquid Separator	-0.000220371		0.000126492	0.000220371
MIX-1	Stream Mixer	-9.98057E-05		0	9.98057E-05
Separator of gas-liquid	Gas-Liquid Separator	0.000164705		-7.48732E-05	-0.000164705
B2	Compressor	-53.1763	75	0	1.17552E-05
B3	Cooler	85.872	100	0	1.12207E-05
B4	Gas-Liquid Separator	-0.00109533		0.000469664	0.00109533
B6	Compressor	-32.7284	75	0	32.7284
B7	Cooler	45.0595	100	0	5.49464E-08
B5	Gas-Liquid Separator	5.60563E-05		2.14498E-06	-5.60563E-05
B9	Gas-Liquid Separator	-2.61702		-6.66195E-06	0.000467737
Heat exchanger 1	Heat Exchanger	-2.53346E-07	80.9505	0	2.53346E-07
TANK-1	Tank	0		0	0
CL-4	Cooler	43	100	0	-1.80635E-07
V-6	Gas-Liquid Separator	0		0	0

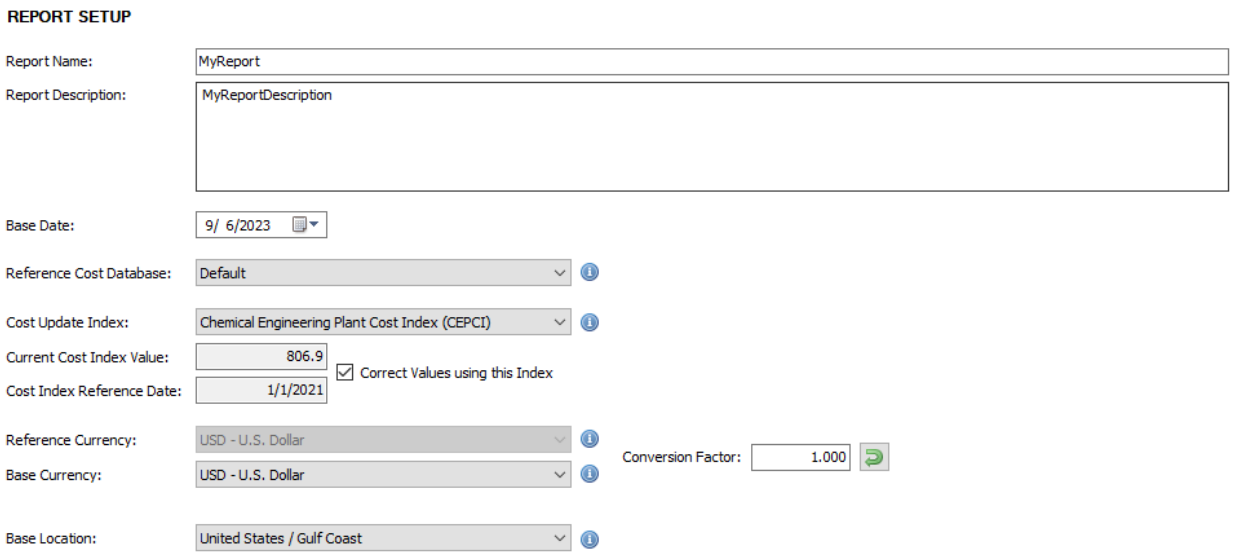
Table 4: Mass and energy balance for streams

Name	Mass Flow (kg/h)	Temperature (°C)	Pressure (bar)	Energy Flow (HP)
30	1984.34	115.412	60	-6661.06
27	29.7683	-150.636	0.996939	-143.948
29	0	80.352	60	0

Name	Mass Flow (kg/h)	Temperature (˚C)	Pressure (bar)	Energy Flow (HP)
waste outlet	15.6596	-150.279	35	-96.8108
24	14.1086	-150.278	35	-47.0888
21	29.7683	-150.279	35	-143.9
20	29.7683	-71.9292	0.996939	-138.948
Gas-out	1984.34	68.0066	60	-6704.06
S15	10.0976	2.57794	0.996939	-60.9996
S11	1989.9	2.57794	0.996939	-6733.53
Ammonia-out	900	-3.37044	3.76987	-1361.53
Compounds together	2000	25	1	-6770.4
S14	2000	2.57794	0.996939	-6794.53
S3	1989.9	85.3419	2.5	-6680.35
S4	1989.9	-40	2.5	-6766.22
S5	1984.29	-38.5681	2.5	-6734.21
S6	5.61165	-40.0001	2.5	-32.0104
S9	1981.63	27.3268	10	-6691.78
S10	1981.63	-38	10	-6736.84
S7	1970.23	-37.9971	10	-6697.99
S8	11.4035	-38.0075	10	-38.8557
Ammonia feed	900	-3.5	3.77	-1385.65
S12	1981.63	-29.992	5	-6724.51
S13	2.65551	-30.0086	5	-7.08212
34	1984.34	68.0066	60	-6704.06
32	1984.34	-37.2394	10	-6745.08
33	1984.34	68.0066	60	-6704.06

5.2.1.1. Cost analysis

The cost analysis is done using DWSIM’s in-built cost estimator for the year 2023. The capital expenditure and optimal expenditure values are calculated in United States dollars (dollars), with each component for optimal expenses and capital expenses calculation having the same cost as that in the United States, setting the base location as India.


REPORT SETUP

Report Name: MyReport

Report Description: MyReportDescription

Base Date: 9/ 6/2023

Reference Cost Database: Default

Cost Update Index: Chemical Engineering Plant Cost Index (CEPCI)

Current Cost Index Value: 806.9

☑ Correct Values using this Index

Cost Index Reference Date: 1/1/2021

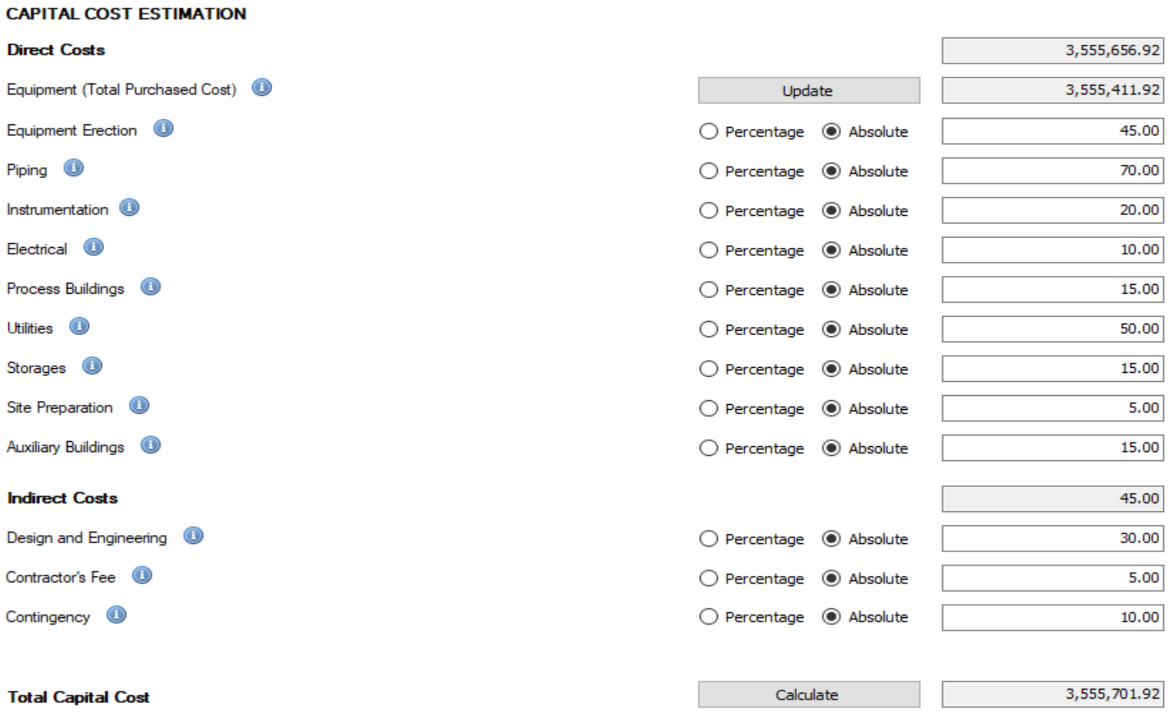
Reference Currency: USD - U.S. Dollar

Base Currency: USD - U.S. Dollar

Conversion Factor: 1.000

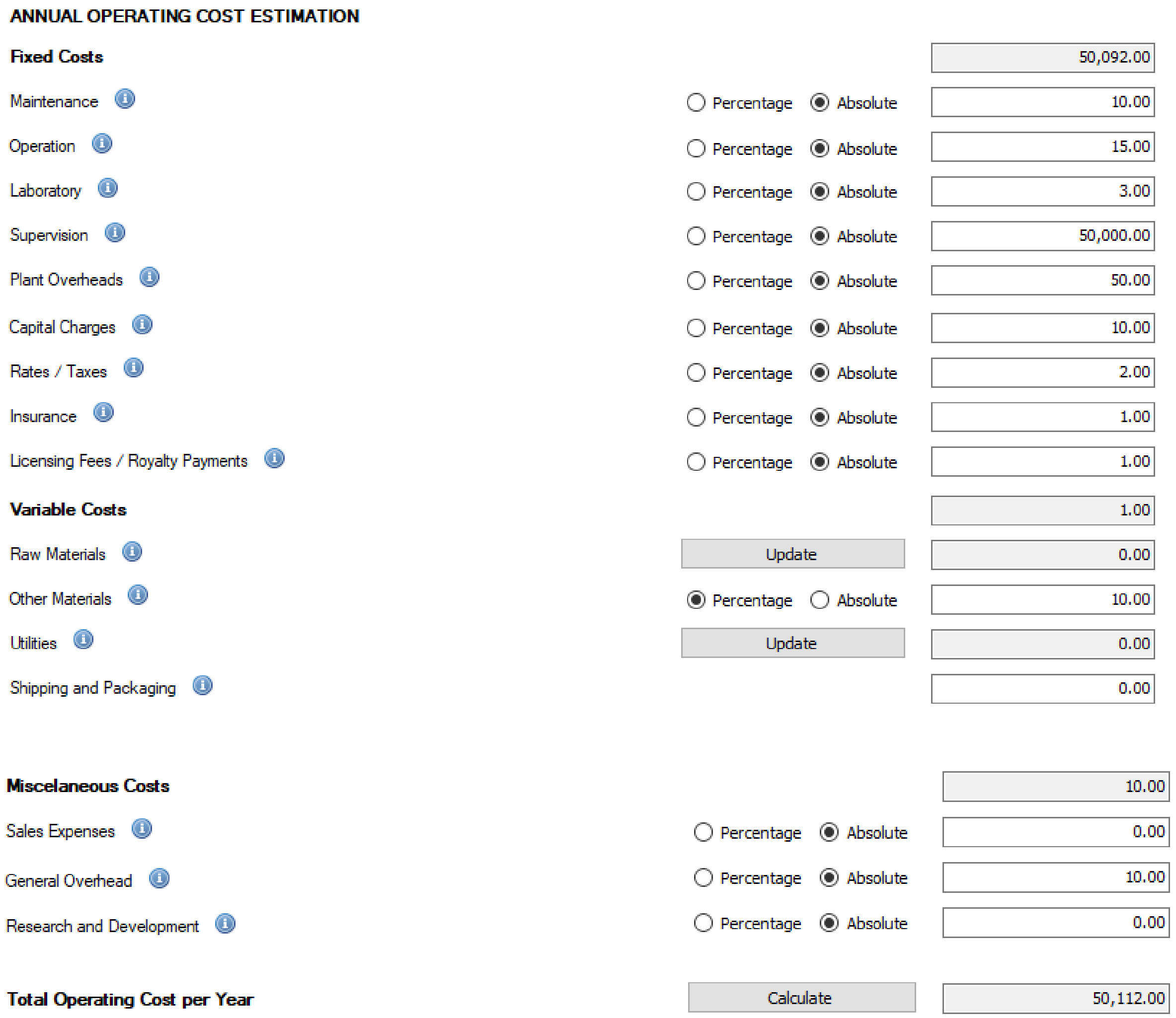
Base Location: United States / Gulf Coast

Figure 6: Parameters setup for cost determination in Capital Cost Estimator of the year 2023 of DWSIM


CAPITAL COST ESTIMATION

Direct Costs		3,555,656.92
Equipment (Total Purchased Cost)	Update	3,555,411.92
Equipment Erection	○ Percentage ● Absolute	45.00
Piping	○ Percentage ● Absolute	70.00
Instrumentation	○ Percentage ● Absolute	20.00
Electrical	○ Percentage ● Absolute	10.00
Process Buildings	○ Percentage ● Absolute	15.00
Utilities	○ Percentage ● Absolute	50.00
Storages	○ Percentage ● Absolute	15.00
Site Preparation	○ Percentage ● Absolute	5.00
Auxiliary Buildings	○ Percentage ● Absolute	15.00
Indirect Costs		45.00
Design and Engineering	○ Percentage ● Absolute	30.00
Contractor's Fee	○ Percentage ● Absolute	5.00
Contingency	○ Percentage ● Absolute	10.00
Total Capital Cost	Calculate	3,555,701.92

Figure 7: Total Capital Cost Estimation (CAPEX)



ANNUAL OPERATING COST ESTIMATION

Fixed Costs		50,092.00
Maintenance	○ Percentage ● Absolute	10.00
Operation	○ Percentage ● Absolute	15.00
Laboratory	○ Percentage ● Absolute	3.00
Supervision	○ Percentage ● Absolute	50,000.00
Plant Overheads	○ Percentage ● Absolute	50.00
Capital Charges	○ Percentage ● Absolute	10.00
Rates / Taxes	○ Percentage ● Absolute	2.00
Insurance	○ Percentage ● Absolute	1.00
Licensing Fees / Royalty Payments	○ Percentage ● Absolute	1.00
Variable Costs		1.00
Raw Materials	Update	0.00
Other Materials	● Percentage ○ Absolute	10.00
Utilities	Update	0.00
Shipping and Packaging		0.00
Miscelaneous Costs		10.00
Sales Expenses	○ Percentage ● Absolute	0.00
General Overhead	○ Percentage ● Absolute	10.00
Research and Development	○ Percentage ● Absolute	0.00
Total Operating Cost per Year	Calculate	50,112.00

Figure 8: Annual operation costs, Miscellaneous Costs and Total Operating Cost per year (OPEX/year)

Total CAPEX and OPEX from the DWSIM results are mentioned as follows, without considering the cost of the tank. Using DWSIM's capital cost estimator plugin for the year 2023 and the location being set as India, the capital cost estimator tool is used to determine the capital cost and optimal expenses, including the cost of ammonia that is used as a coolant in heat exchangers. Also, as the VAT (value-added tax) rate for process equipment and utilities is 13% to import goods in Nepal, many other factors affect the cost estimation so that expenses and costs will increase in the case of Nepal, so the following costs are approximated for expenses.

Table 5: Expenses' parameters

Expenses parameter	Expense value
CAPEX	$17,000,000
OPEX	$10,000,000/year

The tables below show the results generated by the DWSIM simulation for the final outlet stream. The final product stream (gas-out) consists of CO_2 obtained at 99.6% among all product stream constituents that are in the vapor phase, equal by mole fraction as that in the mixed phase. This shows the process proposed above, as shown in Figure 4 can help to use a raw gas mixture consisting of different constituents to capture CO_2 almost completely in a gaseous phase with 99.7%, which can be used for different commercial purposes in industries.

Product composition:

Table 6: Composition of products

Object: Gas-out	
Composition	Mole fraction
Carbon dioxide	0.996354
Water	1.33476E-05
Methane	0.00193581
Ethanol	0.00110049
Methanol	7.37828E-05
Nitrogen	0.000285277
Dimethyl sulfide	0.000176258
Acetaldehyde	6.11301E-05
Ammonia	0
Vapor composition	Mole fraction
Carbon dioxide	0.996354
Water	1.33476E-05
Methane	0.00193581
Ethanol	0.00110049
Methanol	7.37828E-05
Nitrogen	0.000285277
Dimethyl sulfide	0.000176258
Acetaldehyde	6.11301E-05
Total	1

Comparison of product with feed:

For the overall feed/year and product/year calculation, we will assume the feed stream operating for 10 hours/day, 26 days/month, and 12 months/year.

Table 7: Composition of feeds and products

Composition	Feed flow rate (kg/h)	Feed/year	Product/hour	Product/year	Product purity (%)
Carbon dioxide	1979.563	6176236	1779.555	5552211	99.70059
Water	14.91523	46535.51	0.010856	33.86982	0.000608
Methane	1.401977	4374.169	1.401977	4374.167	0.078547
Ethanol	2.288362	7139.689	2.887349	9008.529	0.161765
Methanol	0.854795	2666.961	0.067285	209.928	0.00377
Nitrogen	0.360778	1125.628	0.360778	1125.627	0.020213
Dimethyl Sulphide	0.494416	1542.576	0.494409	1542.556	0.0277
Acetaldehyde	0.121573	379.3092	0.121572	379.3047	0.006811
Total	2000	6240000	1784.899	5568885	100

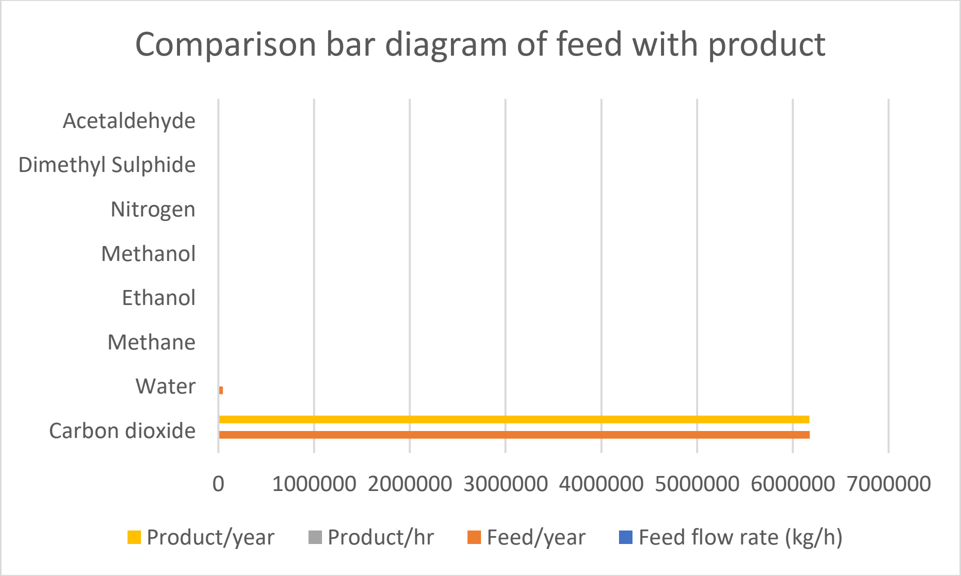


Figure 9: Comparison bar diagram of feed with product

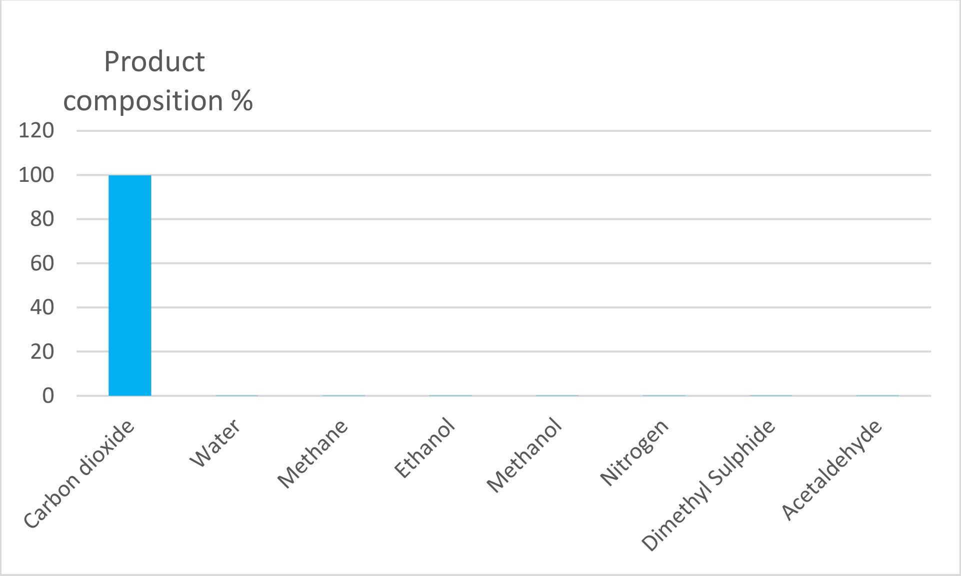


Figure 10: Bar diagram of composition of product

The overall analysis shows that the proposed model is capable of capturing a high quantity of CO_2, but in practical terms, we can expect the plant to capture more than 90% of CO_2, which is a major efficiency improvement from the perspective of the CO_2 capture system. However, the cost of the overall plant setup is very high.

5.2.2. CO_2 capture in the liquid phase

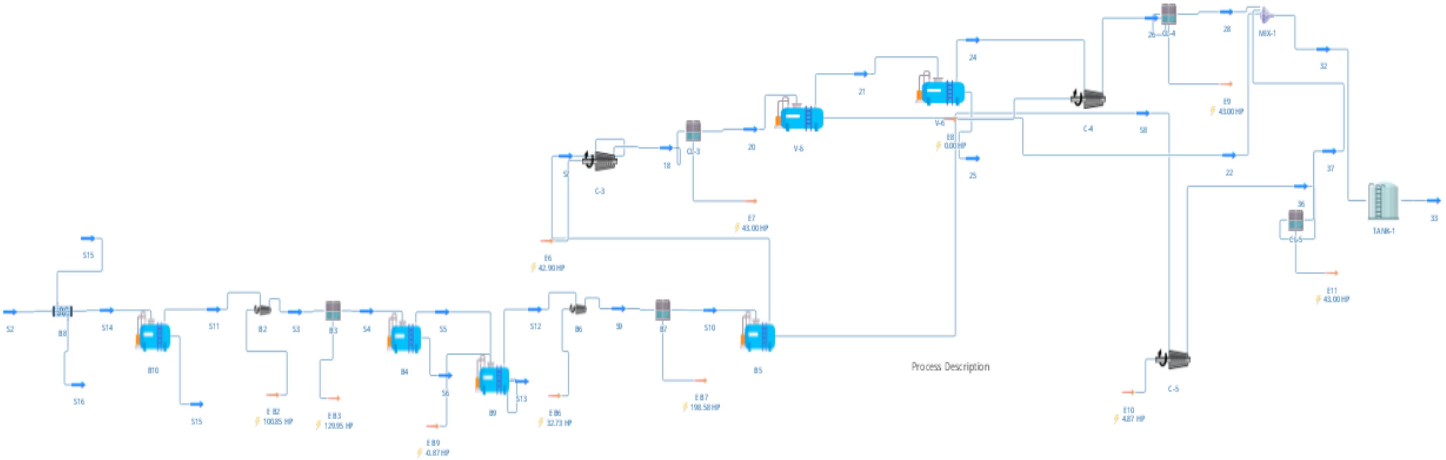


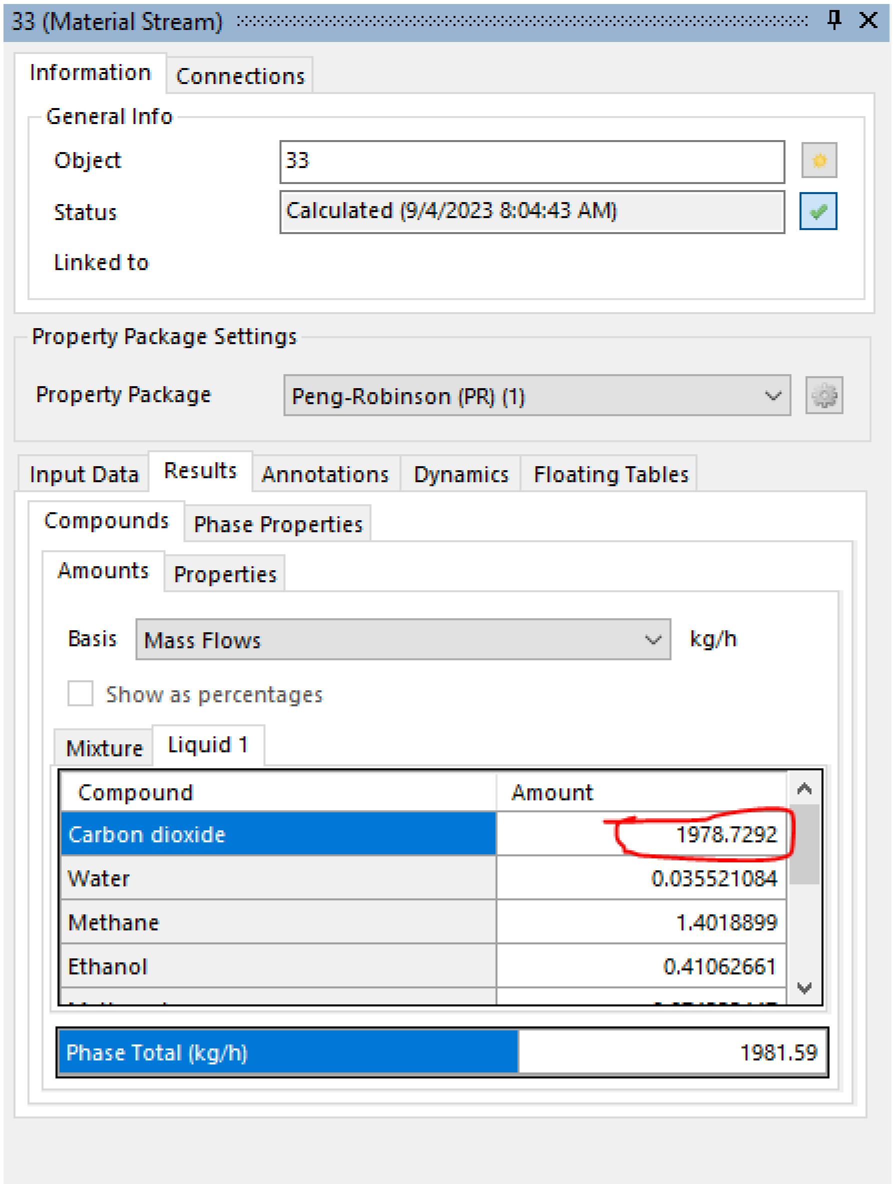
Figure 11: CO_2 capture in liquid phase

Again, 900 kg/hr of ammonia was used in the feed for the only heat exchanger used that acts as a cooler for the stream. The same amount of composition for feed was used as shown in Table 2 through Stream 2. The process that we propose for complete CO_2 capture in the liquid phase is shown in Figure 11. Ammonia is sent on the shell side, and raw gas is sent on the tube side. The inlet conditions for the ammonia and design variables are taken from the available industrial raw gas cooler data.

The PR (Peng-Robinson) property package was used for all components. A vacuum-liquid separator (like B4) is used after the raw gas cooler to separate the liquid in the stream before compression. Five adiabatic compressors with an efficiency of 75% are used before the two flash columns. Five coolers with an efficiency of 100% are used after the flash columns.

In the first flash column, water and methanol are removed from the liquid stream, while carbon dioxide is recovered with other components in the vapor stream. In the second flash column, carbon dioxide is recovered in the liquid stream along with ethanol, dimethyl sulfide, and other components.

The total flow rate of the feed stream was maintained at 2000 kg/h overall for raw gas composition, with temperature and pressure maintained at 25 ˚C and pressure of 1 bar. Liquid carbon dioxide is obtained with 99.72% purity in the stream (33).



Object: 33

Status: Calculated (9/4/2023 8:04:43 AM)

Linked to

Property Package: Peng-Robinson (PR) (1)

Basis: Mass Flows kg/h

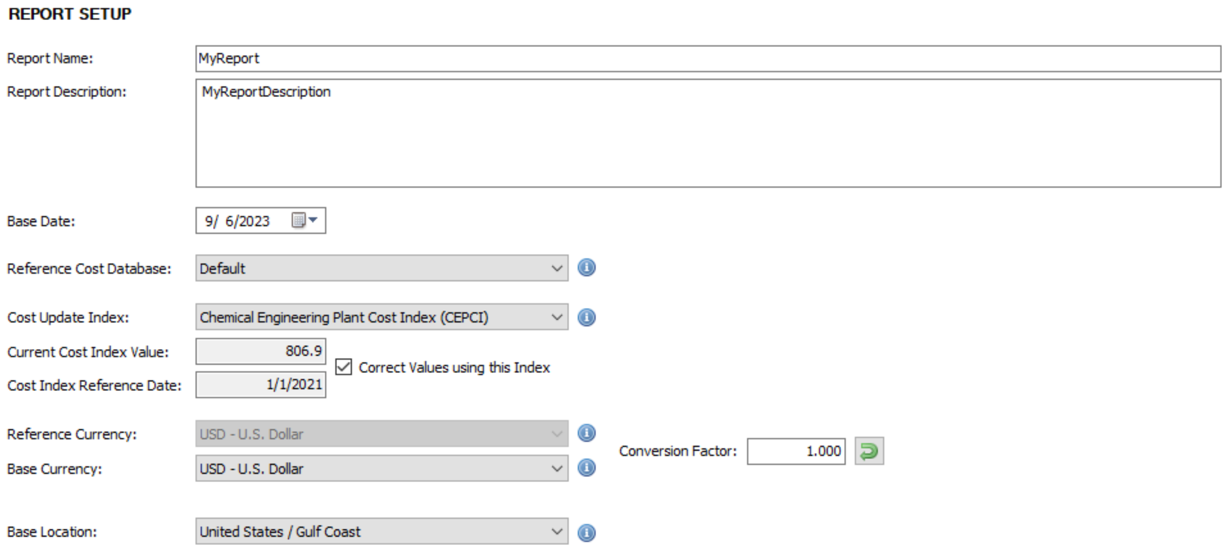
☐ Show as percentages

Compound	Amount
Carbon dioxide	1978.7292
Water	0.035521084
Methane	1.4018899
Ethanol	0.41062661

Phase Total (kg/h): 1981.59

Figure 12: Composition of outflow products in product stream (33)

5.2.2.1. Cost estimation



Report Name: MyReport

Report Description: MyReportDescription

Base Date: 9/ 6/2023

Reference Cost Database: Default

Cost Update Index: Chemical Engineering Plant Cost Index (CEPCI)

Current Cost Index Value: 806.9

Cost Index Reference Date: 1/1/2021

☑ Correct Values using this Index

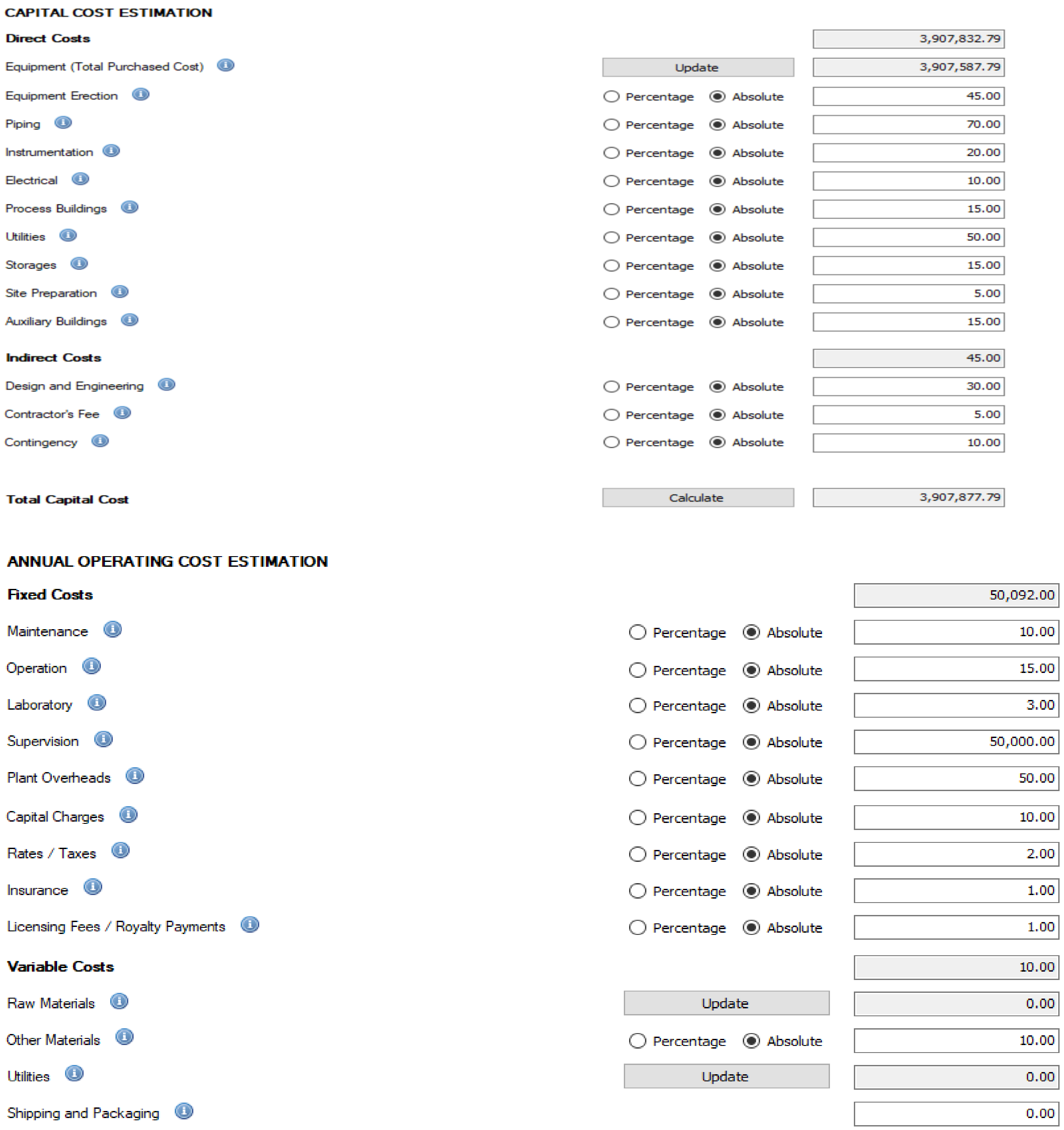
Reference Currency: USD - U.S. Dollar

Base Currency: USD - U.S. Dollar

Conversion Factor: 1.000

Base Location: United States / Gulf Coast

Figure 14: Parameters setup for cost determination in Capital Cost Estimator of the year 2023 of DWSIM



CAPITAL COST ESTIMATION			
Direct Costs			3,907,832.79
Equipment (Total Purchased Cost)	Update		3,907,587.79
Equipment Erection	○ Percentage	● Absolute	45.00
Piping	○ Percentage	● Absolute	70.00
Instrumentation	○ Percentage	● Absolute	20.00
Electrical	○ Percentage	● Absolute	10.00
Process Buildings	○ Percentage	● Absolute	15.00
Utilities	○ Percentage	● Absolute	50.00
Storages	○ Percentage	● Absolute	15.00
Site Preparation	○ Percentage	● Absolute	5.00
Auxiliary Buildings	○ Percentage	● Absolute	15.00
Indirect Costs			45.00
Design and Engineering	○ Percentage	● Absolute	30.00
Contractor's Fee	○ Percentage	● Absolute	5.00
Contingency	○ Percentage	● Absolute	10.00
Total Capital Cost	Calculate		3,907,877.79

ANNUAL OPERATING COST ESTIMATION			
Fixed Costs			50,092.00
Maintenance	○ Percentage	● Absolute	10.00
Operation	○ Percentage	● Absolute	15.00
Laboratory	○ Percentage	● Absolute	3.00
Supervision	○ Percentage	● Absolute	50,000.00
Plant Overheads	○ Percentage	● Absolute	50.00
Capital Charges	○ Percentage	● Absolute	10.00
Rates / Taxes	○ Percentage	● Absolute	2.00
Insurance	○ Percentage	● Absolute	1.00
Licensing Fees / Royalty Payments	○ Percentage	● Absolute	1.00
Variable Costs			10.00
Raw Materials	Update		0.00
Other Materials	○ Percentage	● Absolute	10.00
Utilities	Update		0.00
Shipping and Packaging			0.00

Figure 13: Fixed Costs and Variable costs, Capital Cost (CAPEX)

Miscelaneous Costs			10.00
Sales Expenses	○ Percentage	● Absolute	0.00
General Overhead	○ Percentage	● Absolute	10.00
Research and Development	○ Percentage	● Absolute	0.00
Total Operating Cost per Year	Calculate		50,112.00

Figure 14: OPEX Estimation

Total CAPEX and OPEX from the DWSIM results are mentioned as follows, without considering the cost of the tank. Using DWSIM's capital cost estimator plugin for the year 2023 and the location being set as India, the capital cost estimator tool is used to determine the capital cost and optimal expenses, including the cost of ammonia that is used as a coolant in heat exchangers. Also, as the VAT rate for process equipment and utilities is 13% to import goods in Nepal, many other factors affect the cost estimation due to which expenses and costs will be increased in Nepal, so that the following costs are approximated for expenses:

Table 8: Expenses' parameters

Cost estimation parameter	Cost value
CAPEX	$20,000,000
OPEX	$10,000,000/year

The mass and energy balance at the individual streams and equipment are mentioned below:

Table 9: Mass and energy balance at equipment

Equipment	**Type**	**Energy Consumption (-) / Generation (+) (HP)**	**Efficiency (%)**	**MBR (kg/h)**	**EBR (HP)**
B10	Gas-Liquid Separator	0.000164705		-7.48732E-05	-0.000164705
B2	Compressor	-100.848	75	0	2.41897E-08
B3	Cooler	129.95	100	0	7.50309E-06
B4	Gas-Liquid Separator	-0.00078977		0.00033974	0.00078977
B6	Compressor	-32.7279	75	0	2.88601E-07
B7	Cooler	198.58	100	0	-1.43638E-05
B5	Gas-Liquid Separator	0.000574748		-0.000139333	-0.000574748
B9	Gas-Liquid Separator	0.871412		-2.46812E-06	0.000484518
B8	Heat Exchanger	-2.53346E-07	80.9505	0	2.53346E-07
C-3	Compressor	-42.9019	75	0	-1.47424E-09
CL-3	Cooler	43	100	0	-1.5051E-08
V-5	Gas-Liquid Separator	0		0	0

Equipment	Type	Energy Consumption (-) / Generation (+) (HP)	Efficiency (%)	MBR (kg/h)	EBR (HP)
V-6	Gas-Liquid Separator	0		0	0
C-4	Compressor	0	75	0	0
CL-4	Cooler	43	100	0	1.64882E-06
C-5	Compressor	-4.86949	75	0	8.25775E-08
MIX-1	Stream Mixer	-1.69904E-09		0	1.69904E-09
CL-5	Cooler	43	100	0	1.5196E-09
TANK-1	Tank	0		0	0

Table 10: Mass and energy balance at streams

Name	Mass Flow (kg/h)	Temperature (°C)	Pressure (bar)	Energy Flow (HP)
S15	10.0976	2.57794	0.996939	-60.9996
S11	1989.9	2.57794	0.996939	-6733.53
S16	900	-3.37044	3.76987	-1361.53
S2	2000	25	1	-6770.4
S14	2000	2.57794	0.996939	-6794.53
S3	1989.9	154.148	5	-6632.68
S4	1989.9	-30	5	-6762.63
S5	1984.31	-28.6648	5	-6730.82
S6	5.59112	-30	5	-31.811
S9	1981.59	27.327	10	-6691.64
S10	1981.59	-40	10	-6890.22
S7	726.51	-39.9999	10	-2468.66
S8	1255.08	-40.0003	10	-4421.56
S15	900	-3.5	3.77	-1385.65
S12	1981.59	-29.9981	5	-6724.37
S13	2.72489	-30.009	5	-7.31815
18	726.51	173.287	100	-2425.76
20	726.51	65.9719	100	-2468.76
21	726.51	65.9719	100	-2468.76
22	0	105.166	100	0
24	726.51	65.9719	100	-2468.76
25	0	105.166	100	0
26	726.51	65.9719	100	-2468.76
28	726.51	30.119	100	-2511.76
32	1981.59	-34.977	100	-6971.45

Name	Mass Flow (kg/h)	Temperature (°C)	Pressure (bar)	Energy Flow (HP)
33	1981.59	-34.977	100	-6971.45
36	1255.08	-34.8098	100	-4416.69
37	1255.08	-88.5831	100	-4459.69

Composition in exit stream (33):

Table 11: Composition in exit stream

Object: 33	
Temperature	-34.977
Pressure	100
Mass Flow	1981.59
Molar Flow	45.0849
Volumetric Flow	0.000493011
Mixture Molar Fraction	
Carbon dioxide	0.997261
Water	4.37335E-05
Methane	0.00193826
Ethanol	0.000197703
Methanol	5.1456E-05
Nitrogen	0.000285639
Dimethyl sulfide	0.000163686
Acetaldehyde	5.8084E-05
Ammonia	0
Molar Fraction (Overall Liquid)	
Carbon dioxide	0.997261
Water	4.37335E-05
Methane	0.00193826
Ethanol	0.000197703
Methanol	5.1456E-05
Nitrogen	0.000285639
Dimethyl sulfide	0.000163686
Acetaldehyde	5.8084E-05

Comparison of product with feed:

For the overall feed/year and product/year calculation, we will assume the feed stream operating for 10 hours/day, 26 days/month, and 12 months/year.

Table 12: Comparison of product with feed

Components	Feed flow rate (kg/hour)	Feed/year	Product (kg/hour)	Product/year	Product purity (%)
Carbon dioxide	1979.563	6176236	1978.727	6173629	99.83588
Water	14.91523	46535.51	0.035521	110.8258	0.001792
Methane	1.401977	4374.169	1.40189	4373.896	0.070732
Ethanol	2.288362	7139.689	0.410627	1281.155	0.020718
Methanol	0.854795	2666.961	0.074333	231.9204	0.00375
Nitrogen	0.360778	1125.628	0.360757	1125.562	0.018202
Dimethyl Sulphide	0.494416	1542.576	0.854535	2666.148	0.043115
Acetaldehyde	0.121573	379.3092	0.115361	359.9261	0.00582
Total	2000	6240000	1981.98	6183778	100

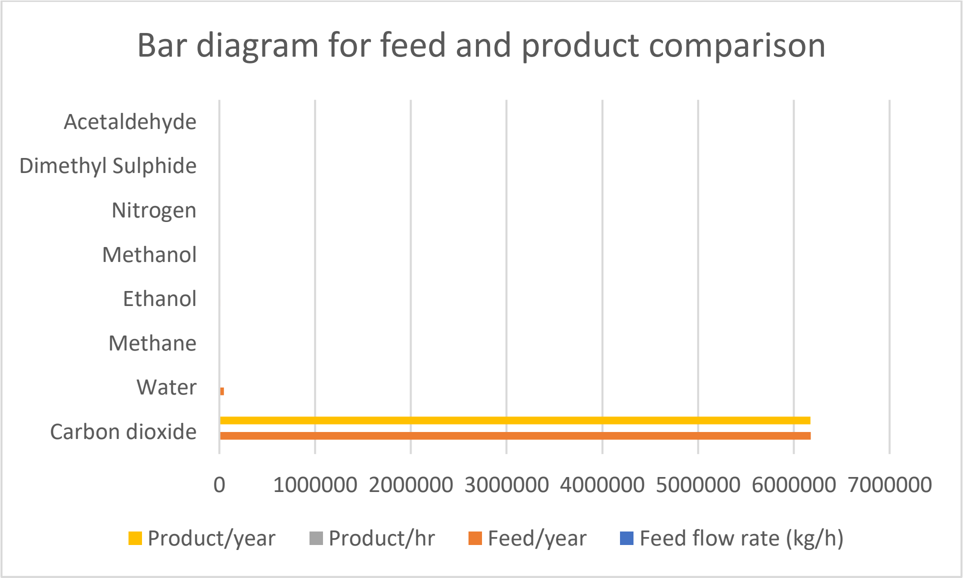


Figure 15: Bar diagram of feed and product

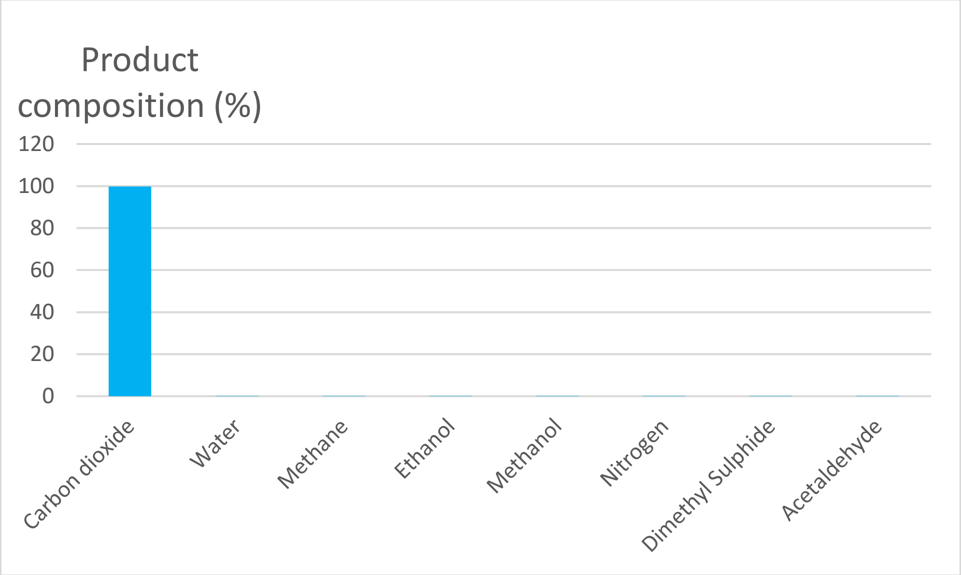


Figure 16: Bar diagram for product composition

The above results show that the proposed model in Figure 11 is sufficient to generate CO_2 from raw gases produced in different industries. The CAPEX and OPEX involved are high, but the liquid form of CO_2 is highly useful to generate high income through various methods like the production of methanol and urea.

5.3. Model for flue gas from Cement industries

Flue gas from the cement industry is a complex mixture of gases and particulate matter that is emitted into the atmosphere during the cement production process. The main components of flue gas from cement plants are carbon dioxide (CO_2), nitrogen oxides (NOx), sulfur dioxide (SO_2), and particulate matter (PM).

Flue gas from cement plants can have a significant impact on the environment and human health. CO_2 is a greenhouse gas that contributes to climate change. NOx and SO_2 can react with other pollutants in the atmosphere to form ground-level ozone and smog, which can cause respiratory problems, heart disease, and other health problems. PM can also cause respiratory problems and other health problems, and it can also reduce visibility.

There are a number of ways to reduce emissions of pollutants from cement plants. One way is to improve the efficiency of the cement production process. Another way is to use cleaner fuels, such as natural gas, instead of coal. Cement plants can also install pollution control equipment, such as electrostatic precipitators and scrubbers, to remove pollutants from flue gas.

In recent years, the cement industry has made significant progress in reducing emissions of pollutants. However, there is still more work to be done. The cement industry continues to develop new technologies to reduce emissions and improve the environmental performance of cement production in developed countries, but in the case of developing countries, the waste flue gases from cement industries are producing a major effect on the ozone layer of the Earth and are a major contributor to climate change.

Here are some specific examples of how the cement industry is reducing emissions of pollutants:

CO_2: The cement industry is working to reduce CO_2 emissions by using alternative fuels, such as biomass and waste materials, in the cement production process. The cement industry is also developing new technologies to capture and store CO_2.

NOx: The cement industry is reducing NOx emissions by using low-NOx burners and other combustion technologies. The cement industry is also developing new technologies to remove NOx from flue gas.

SO_2: The cement industry is reducing SO_2 emissions by using low-sulfur fuels and by installing flue gas desulfurization (FGD) systems. FGD systems remove SO_2 from flue gas by reacting it with limestone or other alkaline reagents.

PM: The cement industry is reducing PM emissions by the installation of electrostatic precipitators and other particulate control devices. Electrostatic precipitators use an electric field to remove PM from flue gas.

The cement industry is committed to reducing emissions of pollutants and improving the environmental performance of cement production in developed countries, but in the context of developing countries like Nepal, CO_2 emissions are a major problem. Since developing countries like Nepal lack enough technicians, resources, capital, and awareness of the effects of such industrial deposits, the industrial flue gases are being released without proper treatment. CO_2 capture by compression followed by cooling at high pressure can lead to the development of a novel technology that can contribute to reducing such pollutants by a significant amount.

In order to estimate the feasibility of cryogenic CO_2 capture in the context of developing countries like Nepal, the Sarbottam cement industry, which is one of the largest cement industries in Nepal, is selected. The following models are used to determine the best combination of different types of equipment and the cost estimation of the obtained results for the input data of flue gas from [34].

Figure 17: Location of the Sarbottam cement's industrial plant

Devkota et al., in their research [34], estimated the economics and feasibility of building a carbon capture pant based on the membrane separation method using the aspen plus model for the flue gas composition of the Sarbottam Cement Industry. The following data on flue gas composition generated by the Sarbottam cement industry has been used by the authors in their techno-economic analysis:

Table 13: Composition of flue gas

Variable	Value	Unit
Flow rate	64.4	kg/s
Temperature	565	K
Pressure	1	bar
Composition [%]	Moles	Mass
CO_2	10.21	15.18
CO	0.016	0.000795
O_2	0.015	0.000131
N_2	88.9	84.14

5.3.1. Single-stage cryogenic compression

The same data can be used for techno-economic analysis and feasibility estimation of estimation of Cryogenic compression and Separation process for CO_2 capture using the following model developed in DWSIM software:

The following model was built in DWSIM and is used to assess the efficiency of the cryogenic compression and separation process:

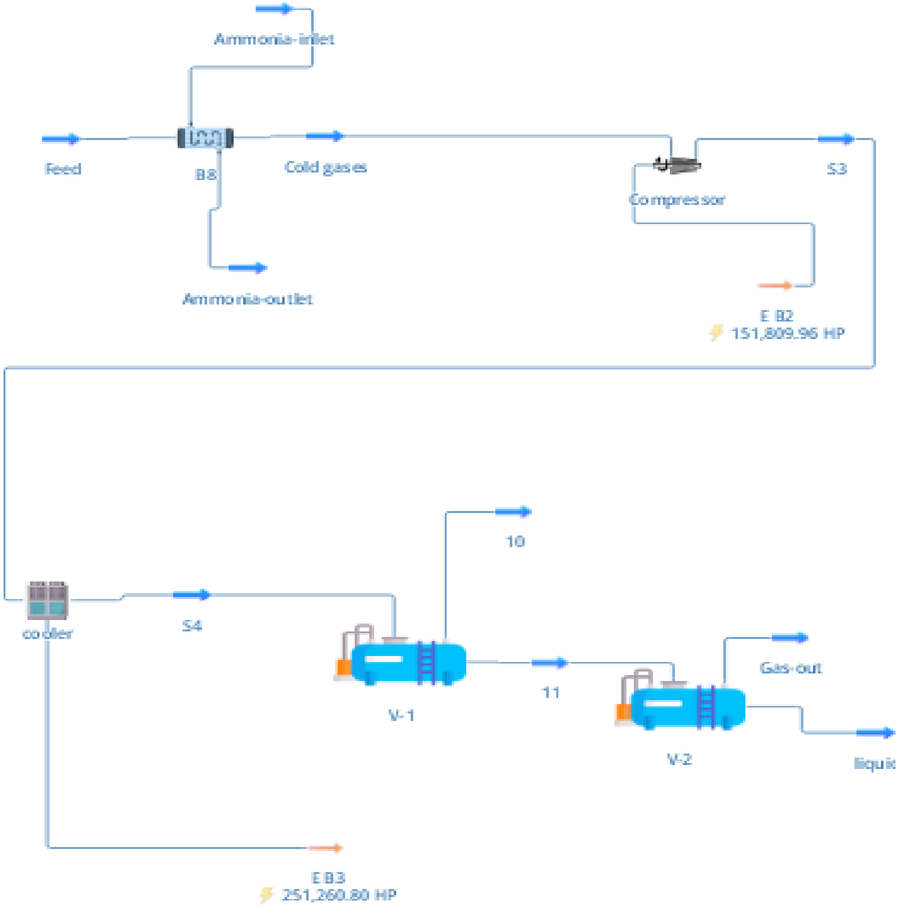


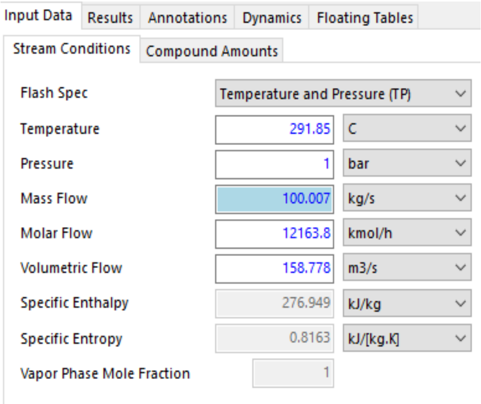
Figure 18: Capture of CO2 using cryogenic compression and separation process

In order to capture CO_2 completely in the liquid phase, 1 kg/s of ammonia was used in the feed for the only heat exchanger that acts as a cooler for the stream. The same amount of composition for feed was used as shown in Table 12 through Stream 2. The process that we propose for complete CO_2 capture in the liquid phase is shown in Figure 11. Ammonia is sent on the shell side, and raw gas is sent on the tube side. The inlet conditions for the ammonia and design variables are taken from the available flue gas data.

The PR (Peng-Robinson) property package was used for all components. Vapor-liquid separators (like V-1 and V-2) are used after the raw gas cooler to separate the liquid in the stream before compression. Five adiabatic compressors with an efficiency of 75% are used before the two flash columns. Five coolers with an efficiency of 100% are used after the flash columns.

In the first flash column, water and methanol are removed from the liquid stream, while carbon dioxide is recovered with other components in the vapor stream. In the second flash column, carbon dioxide is recovered in the liquid stream along with ethanol, dimethyl sulfide, and other components.

The total flow rate of the feed stream was maintained at 12163.8 kmol/h for the overall raw gas composition, with temperature and pressure maintained at 25 ˚C and pressure of 1 bar. The inlet and various components used are mentioned in Figure 19 and Table 13 below:



Flash Spec: Temperature and Pressure (TP)
Temperature: 291.85 C
Pressure: 1 bar
Mass Flow: 100.007 kg/s
Molar Flow: 12163.8 kmol/h
Volumetric Flow: 158.778 m3/s
Specific Enthalpy: 276.949 kJ/kg
Specific Entropy: 0.8163 kJ/[kg.K]
Vapor Phase Mole Fraction: 1

Figure 19: Properties of the feed

The total composition of the liquid components at the outlet stream (liquid) are as follows:

Table 14: Liquid component at outlet stream

Carbon dioxide	14.828293 Kg
Water	7.950119E-05 Kg
Oxygen	0.0076318102 Kg
Hydrogen	3.4436648E-06 Kg
Nitrogen	0.067058199 Kg
Ammonia	0 Kg
Carbon monoxide	1.3680587E-05 Kg

Similarly, the total composition of gaseous products left in the outlet stream are as follows:

Table 15: Gaseous products at the outlet stream

Carbon dioxide	0.0026322417 Kg
Water	6.9531707E-16 Kg
Oxygen	0.0066276709 Kg
Hydrogen	0.00309597 Kg
Nitrogen	0.9874622 Kg
Ammonia	0 Kg
Carbon monoxide	0.00018192033 Kg

The compressor used had a pressure of 30 bar and an efficiency of 75% with a power requirement of 151,810 HP.

The above analysis and results in Tables 15 and 16 show that the proposed system is effective enough to capture CO_2 in the liquid phase. The following data shows the features of the various components used:

Table 16: Mass and energy balance at equipment

Equipment	**Type**	**Energy Consumption (-) / Generation (+) (HP)**	**Efficiency (%)**	**MBR (kg/s)**	**EBR (HP)**
Compressor	Compressor	-151810	75	0	6.08925E-07
cooler	Cooler	251261	100	0	-0.0513208
V-2	Gas-Liquid Separator	-2.37199E-05		-8.80007E-11	2.37199E-05
V-1	Gas-Liquid Separator	2.69198		-8.0731E-05	-2.69198
B8	Heat Exchanger	-3.53822E-05	65.4857	0	3.53822E-05

Table 17: Mass and energy balance at used streams

Name	**Mass Flow (kg/s)**	**Temperature(°C)**	**Pressure (bar)**	**Energy Flow (HP)**
Ammonia-outlet	1	-2.73179	3.67	-3762.07
Feed	100.007	291.85	1	-146971
Cold gases	100.007	279.583	0.997137	-148752

Name	**Mass Flow (kg/s)**	**Temperature(°C)**	**Pressure (bar)**	**Energy Flow (HP)**
S3	100.007	1226.85	30	3058.43
S4	100.007	-200	30	-248202
liquid	14.9031	-200	30	-193347
10	85.1036	-200	30	-54857.9
11	14.9031	-200	30	-193347
Ammonia-inlet	1	-3.5	3.77	-5542.61
Gas-out	1.06028E-05	-200	30	-0.00683463

The DWSIM Capital Cost Estimator for the year 2023 tool was used to determine the capital cost (CAPEX) of the plant that can be calculated on the basis of the proposed model in Figure 18. The total capital cost that involves the following items of expenses, as mentioned in Table 17 below, setting the base location of the plant as India, which is a border country with Nepal, showed the total capital cost (CAPEX) to be $110,824,530.82, which can be approximated to $112,000,000. The approximated cost is predicted to be higher due to inflation, transportation, shipping, and other causes that make the overall cost quite higher in Nepal for building the plant compared to India.

Table 18: Expenses' parameters

Cost Category	Percentage
Direct Costs	
Equipment (Total Purchased Cost)	30%
Equipment Erection	10%
Piping	3%
Instrumentation	3%
Electrical	10%
Process Buildings	4%
Utilities	5%
Site Preparation and safety	10%
Auxiliary Buildings	3%
Indirect Costs	
Design and Engineering	8%
Contractor's Fee	7%
Contingency	7%

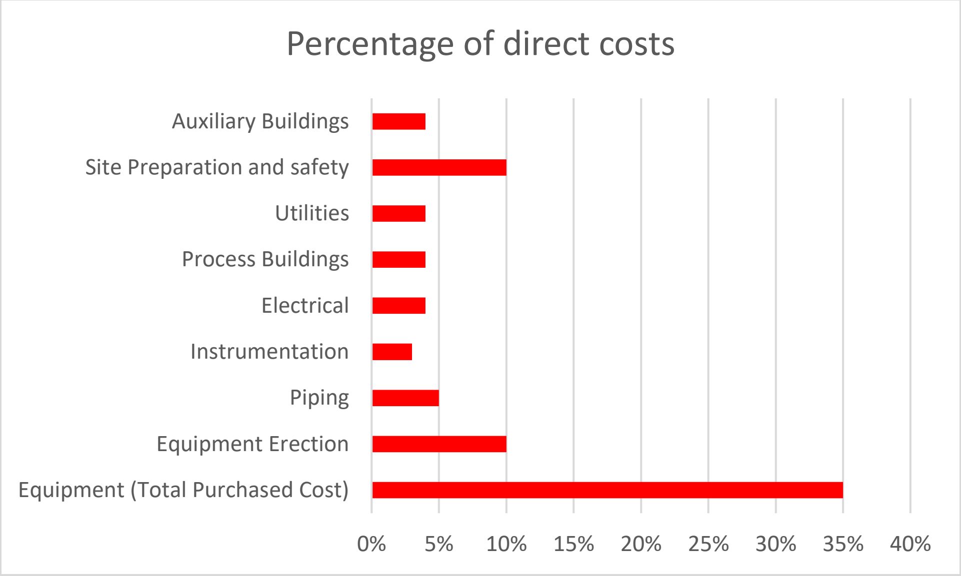


Figure 20: Percentage of direct cost items

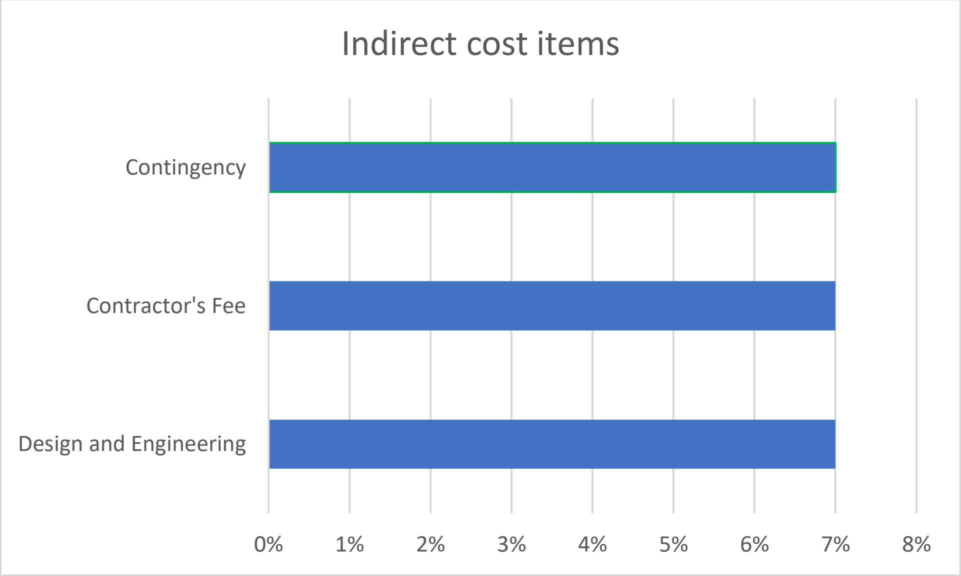


Figure 21: Percentage of indirect cost items

Similarly, the OPEX value for various items like:

Fixed Costs:

- Maintenance costs
- Operation
- Laboratory
- Supervision

- Plant overheads
- Capital charges
- Rates/Taxes
- Insurance
- Licensing fees/ Royalty payments

Variable costs:

- Raw materials
- Other materials

Miscellaneous costs:

- Utilities
- Shipping and packaging

Estimation of the cost through these items showed a cost of $55,241,699.64/year as OPEX for this plant consisting of single-stage cryogenic compression, including the cost of ammonia used for the total year as coolant. This cost was calculated by setting the base location as India in the DWSIM Capital Cost Estimator for the year 2023. This cost can be approximated at $56,000,000/year for the case of Nepal since the cost gets increased due to factors like shipping costs, the inflation rate, and transportation, making the cost quite higher than that in India.

The sensitivity analysis was performed based on the variation between the input mass flow rate at the 'Feed' section for individual compound amounts, which decreased and increased within a certain range, as mentioned in Table 18, along with the mass flow rate of ammonia at the 'Ammonia-Inlet'. This caused the generation of varied product mass flow rates of compounds in the 'product' stream, as shown in Table 18 and Figure 22.

Table 19: Comparison of feed and product

Ammonia-inlet - Mass Flow (kg/s)	Feed - Mass Flow (kg/s)	liquid - Mass Flow (Liquid 1) / Carbon dioxide (kg/s)
0	50	7.41366
0	75	11.1205
0	100	14.8273
0	125	18.5341
0	150	22.241

1.25	50	7.41366
1.25	75	11.1205
1.25	100	14.8273
1.25	125	18.5341
1.25	150	22.241
2.5	50	7.41366
2.5	75	11.1205
2.5	100	14.8273
2.5	125	18.5341
2.5	150	22.241
3.75	50	7.41366
3.75	75	11.1205
3.75	100	14.8273
3.75	125	18.5341
3.75	150	22.241
5	50	7.41366
5	75	11.1205
5	100	14.8273
5	125	18.5341
5	150	22.241

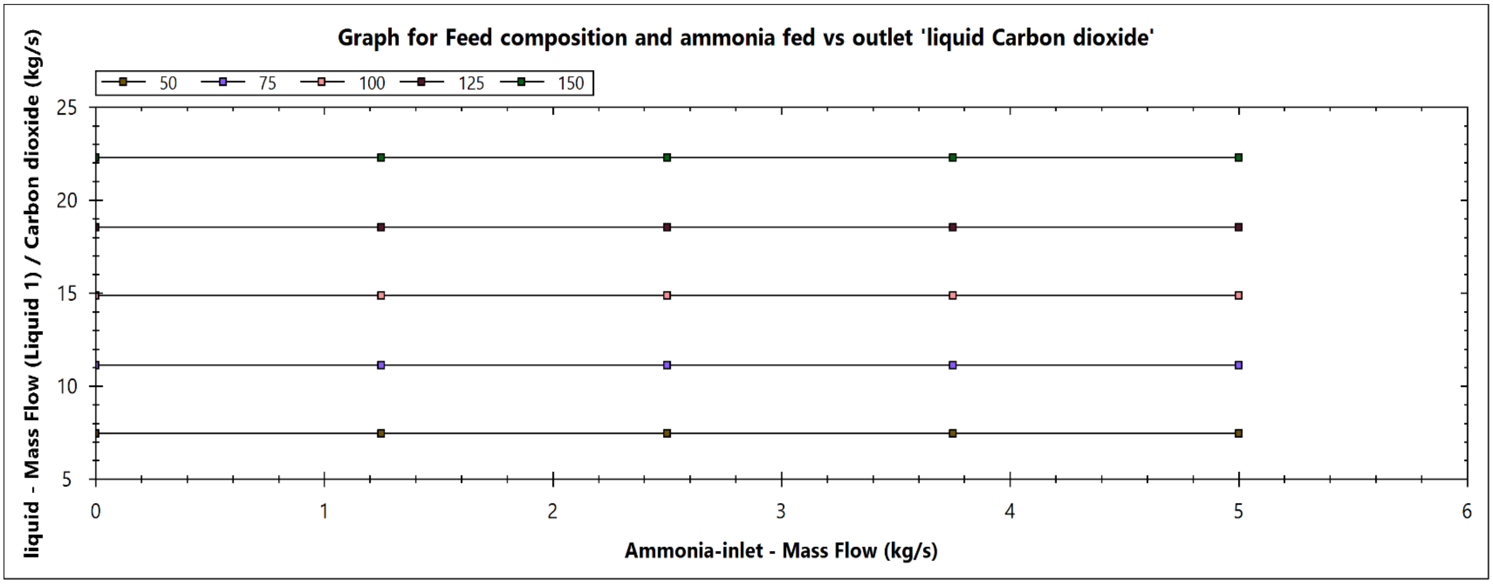


Figure 22: Graph for sensitivity analysis for ammonia fed vs outlet's liquid CO_2

Again, to assess the effect of a change in compressor pressure and the cooler's outlet temperature on the liquid CO_2 production in the final liquid stream 'liquid', the compressor's pressure was changed between 2000000 Pa to 3500000 Pa, and the cooler's outlet temperature was changed between range -100 ˚C. The outlet liquid CO_2 composition was determined for the 'liquid' stream as mentioned in the table and figure below:

Table 20: Results of sensitivity analysis

Compressor - Pressure Increase (Pa)	cooler - Outlet Temperature (˚C)	liquid - Mass Flow (Liquid 1) / Carbon dioxide (kg/s)
2000000	-100	11.294
2000000	-137.5	14.9533
2000000	-175	13.9078
2000000	-212.5	15.0715
2000000	-250	15.18
2375000	-100	11.294
2375000	-137.5	14.9533
2375000	-175	13.9078
2375000	-212.5	15.0715
2375000	-250	15.18
2750000	-100	11.294
2750000	-137.5	14.9533
2750000	-175	13.9078
2750000	-212.5	15.0715
2750000	-250	15.18
3125000	-100	11.294
3125000	-137.5	14.9533
3125000	-175	13.9078
3125000	-212.5	15.0715
3125000	-250	15.18
3500000	-100	11.294
3500000	-137.5	14.9533
3500000	-175	13.9078
3500000	-212.5	15.0715
3500000	-250	15.18

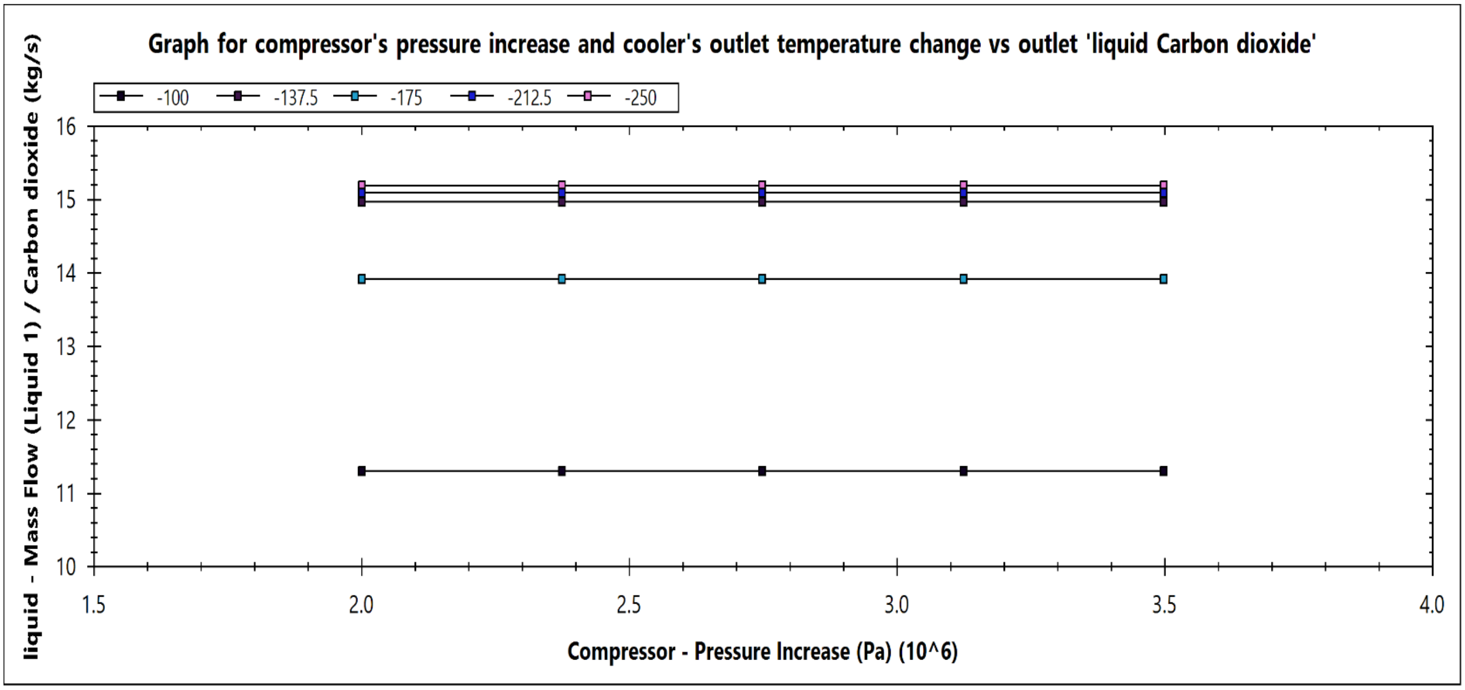


Figure 23: Compressor’s pressure increase and cooler’s outlet temperature vs liquid CO_2 produced Compressor’s pressure increase and cooler’s outlet temperature vs liquid CO_2 produced

From the above sensitivity study, we find that the value of the mass flow rate of liquid product CO_2 at stream ‘liquid’ varies linearly within certain ranges of values of the compressor’s pressure increase and increase in the cooler’s outlet temperature.

5.3.2. Two-stage compression and cooling

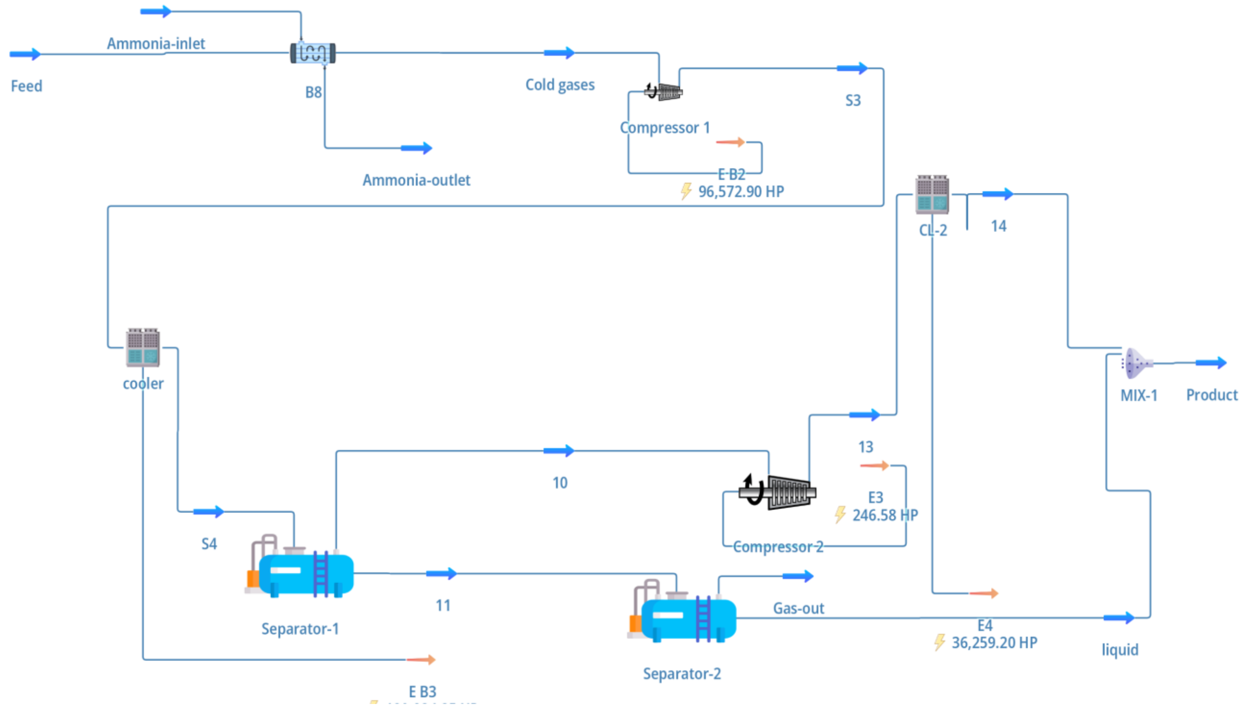
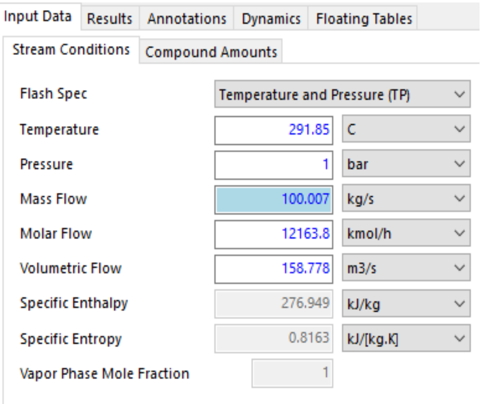


Figure 24: Two-stage compression and cooling

In order to capture CO_2 completely in the liquid phase, 1 kg/s of ammonia was used in the feed for the only heat exchanger that acts as a cooler for the stream. The PR thermodynamic property for individual components was used. The same amount of composition for feed was used as shown in Table 12 through Stream 'Ammonia-Inlet'. Ammonia is sent on the shell side, and raw gas is sent on the tube side. The inlet conditions for the ammonia and design variables are taken from the available industrial flue gas data.

The PR (Peng-Robinson) property package was used for all components. Vapor-liquid separators (like Separator-1 and Separator-2) are used after the raw gas cooler to separate the liquid in the stream before compression. Five adiabatic compressors with an efficiency of 75% are used before the two flash columns. Five coolers with an efficiency of 100% are used after the flash columns.

In the first flash column, water and methanol are removed from the liquid stream, while carbon dioxide is recovered with other components in the vapor stream. In the second flash column, carbon dioxide is recovered in the liquid stream along with ethanol, dimethyl sulfide, and other components.



Flash Spec: Temperature and Pressure (TP)
Temperature: 291.85 C
Pressure: 1 bar
Mass Flow: 100.007 kg/s
Molar Flow: 12163.8 kmol/h
Volumetric Flow: 158.778 m3/s
Specific Enthalpy: 276.949 kJ/kg
Specific Entropy: 0.8163 kJ/[kg.K]
Vapor Phase Mole Fraction: 1

Figure 25: Inlet conditions for stream feed

Similarly, the compounds and their mass flow rate in (kg/s) for stream 'feed' are as follows:

Table 21: Mass flow rate of fed compounds

Carbon dioxide	15.18
Water	7.95E-05
Oxygen	0.652
Hydrogen	0.019
Nitrogen	84.14
Ammonia	0
Carbon monoxide	0.0155

The hot fluid outlet temperature was set to -3 ˚C for the ammonia-fed heat exchanger 'B8' which is shown in Figure 24.

The following properties were used or obtained for respective streams for the model in Figure 24.

Table 22: Mass and energy balance for equipment used

Equipment	**Type**	**Energy Consumption (-) / Generation (+) (HP)**	**Efficiency (%)**	**MBR (kg/s)**	**EBR (HP)**
Compressor 2	Compressor	-246.58	75	0	-9.96498E-06
CL-2	Cooler	36259.2	100	0	0.0001818
B8	Heat Exchanger	38834.5	100	0	-38834.5

Equipment	Type	Energy Consumption (-) / Generation (+) (HP)	Efficiency (%)	MBR (kg/s)	EBR (HP)
Separator-1	Gas-Liquid Separator	5.2059		-0.00015616	-5.2059
Separator-2	Gas-Liquid Separator	-0.000338939		9.79182E-09	0.000338939
cooler	Cooler	120834	100	0	-0.0439685
Compressor 1	Compressor	-96572.9	75	0	3.61078E-08
MIX-1	Stream Mixer	0.0574433		0	-0.0574433

Table 23: Mass and energy balance at streams

Equipment	Type	Energy Consumption (-) / Generation (+) (HP)	Efficiency (%)	MBR (kg/s)	EBR (HP)
Compressor 2	Compressor	-246.58	75	0	-9.96498E-06
CL-2	Cooler	36259.2	100	0	0.0001818
B8	Heat Exchanger	38834.5	100	0	-38834.5
Separator-1	Gas-Liquid Separator	5.2059		-0.00015616	-5.2059
Separator-2	Gas-Liquid Separator	-0.000338939		9.79182E-09	0.000338939
cooler	Cooler	120834	100	0	-0.0439685
Compressor 1	Compressor	-96572.9	75	0	3.61078E-08
MIX-1	Stream Mixer	0.0574433		0	-0.0574433

Also, the mass flow rate in kg/sec of the individual components of the product stream in liquid phase are as follows:

Table 24: Mass flow rate for product components

Carbon dioxide	14.896406
Water	7.9504214E-05
Oxygen	0.0068339291
Hydrogen	2.6129361E-06
Nitrogen	0.053290699
Ammonia	0

Carbon monoxide	1.0934996E-05

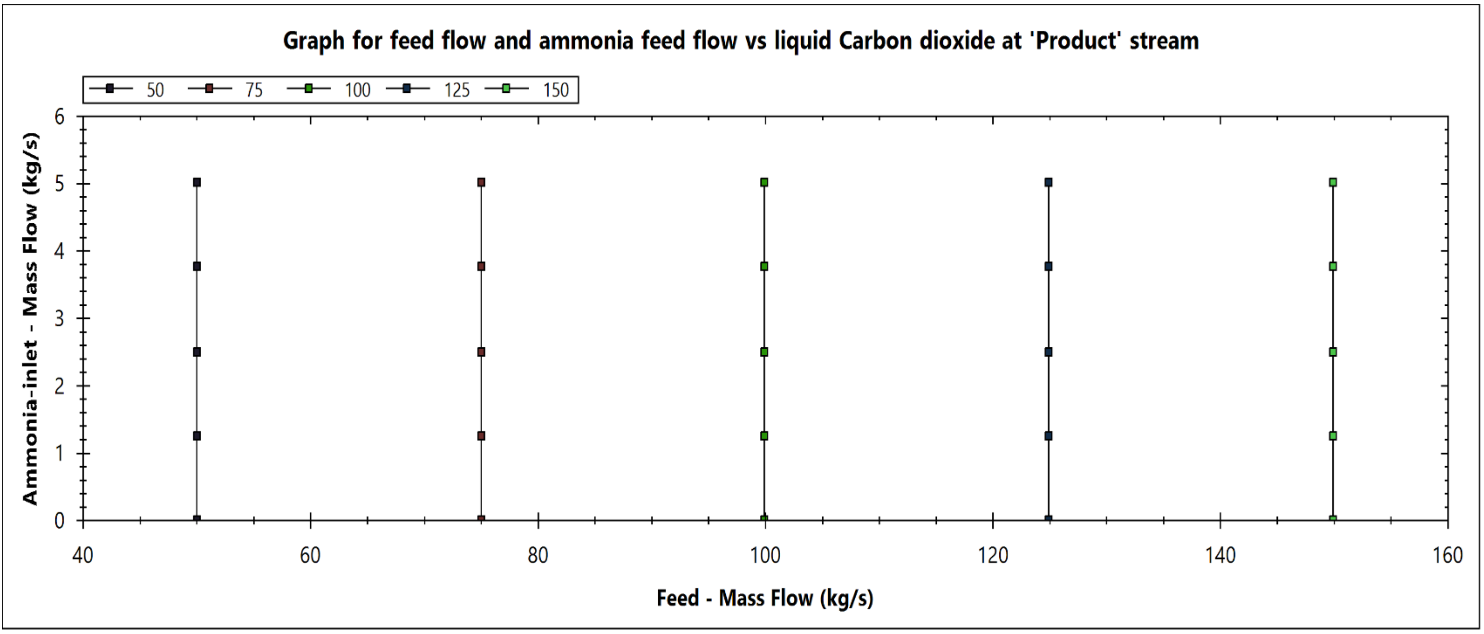


Figure 26: Graph for feed flow and ammonia feed flow vs liquid CO_2 produced

The following data were obtained for the sensitivity analysis when the input values of ammonia inlet and feed flow rate at the ‘Feed’ stream were varied so that the product composition changes at the ‘liquid’ stream for liquid carbon dioxide:

The sensitivity analysis was performed as shown in Figure 26 above, and the plot showed the outlet ‘Product’ stream’s CO_2 composition varied linearly with the inlet’s ammonia mass flow rate at the ‘Ammonia-inlet’ stream and ‘Feed’ stream’s flue gas composition.

Similarly, when the power required for ’Compressor 1’ and the heat removed ‘COOLER’ were used to check the variation of product liquid CO_2 at the ‘Product’ stream, the following results and graph plot were obtained:

Table 25: Sensitivity analysis’s results

Compressor - Pressure Increase (Pa)	cooler - Outlet Temperature (°C)	liquid - Mass Flow (Liquid 1) / Carbon dioxide (kg/s)
2000000	-100	11.294

2000000	-137.5	14.9533
2000000	-175	13.9078
2000000	-212.5	15.0715
2000000	-250	15.18
2375000	-100	11.294
2375000	-137.5	14.9533
2375000	-175	13.9078
2375000	-212.5	15.0715
2375000	-250	15.18
2750000	-100	11.294
2750000	-137.5	14.9533
2750000	-175	13.9078
2750000	-212.5	15.0715
2750000	-250	15.18
3125000	-100	11.294
3125000	-137.5	14.9533
3125000	-175	13.9078
3125000	-212.5	15.0715
3125000	-250	15.18
3500000	-100	11.294
3500000	-137.5	14.9533
3500000	-175	13.9078
3500000	-212.5	15.0715
3500000	-250	15.18

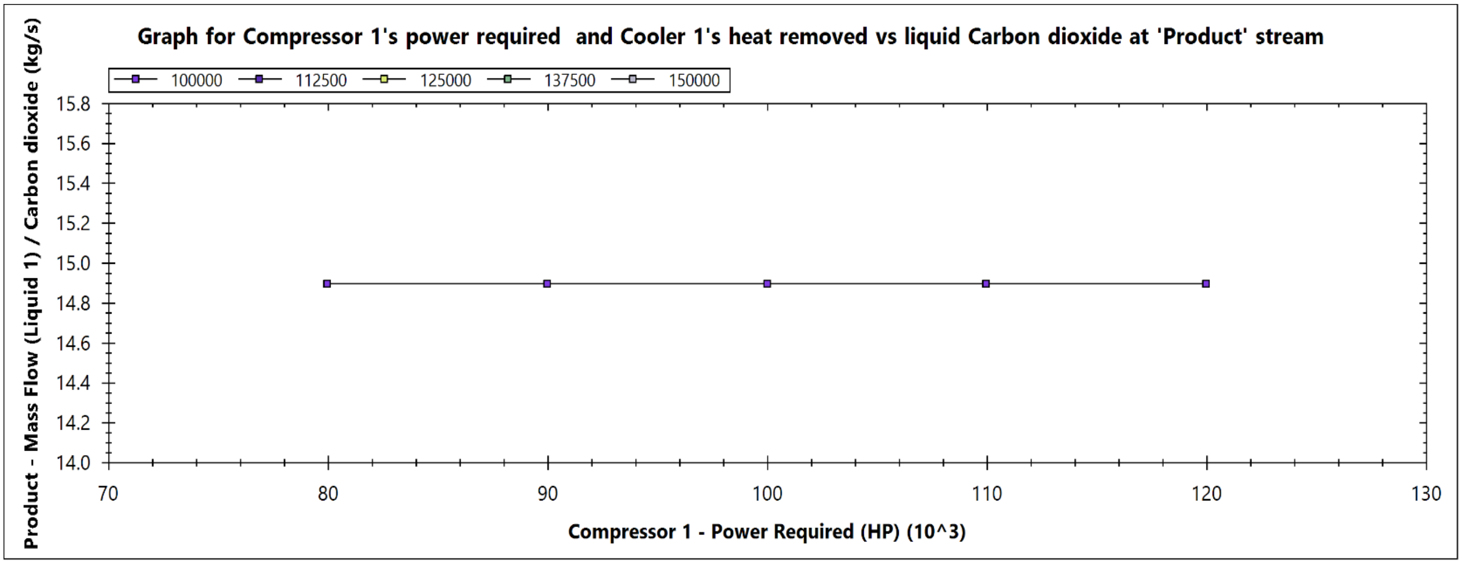


Figure 27: Graph for compressor's power required and cooler's heat removed vs product liquid CO_2

Similarly, the value of Compressor-2's power required and CL-2's temperature difference was varied with Product-Mass Flow's liquid CO_2 component, and the following results were obtained:

Table 26: Sensitivity analysis's results

Compressor 2 - Power Required (HP)	CL-2 - Temperature Difference (K.)	Product - Mass Flow (Liquid 1) / Carbon dioxide (kg/s)
200	-150	15.174
200	-87.5	13.8309
200	-25	14.0709
200	37.5	5.22297
200	100	0
225	-150	15.174
225	-87.5	13.8309
225	-25	14.0709
225	37.5	5.22297
225	100	0
250	-150	15.174
250	-87.5	13.8309

250	-25	14.0709
250	37.5	5.22297
250	100	0
275	-150	15.174
275	-87.5	13.8309
275	-25	14.0709
275	37.5	5.22297
275	100	0
300	-150	15.174
300	-87.5	13.8309
300	-25	14.0709
300	37.5	5.22297
300	100	0

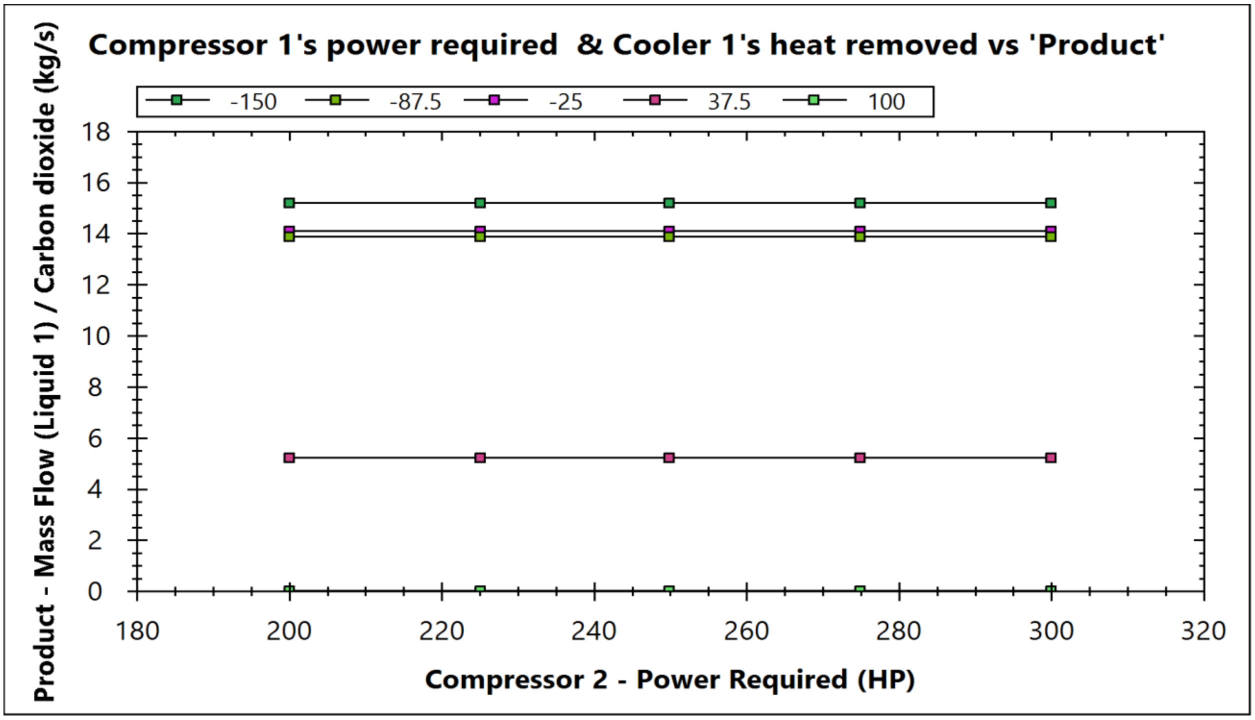


Figure 28: Graph for compressor 1’s power required and cooler 1’s heat removed vs product

As shown by the above Table 25 and Figure 28, the liquid CO_2 composition is affected by a certain value of the compressor’s pressure and the cooler’s outlet temperature.

Similarly, the power required for compressors 1 and 2 was varied as independent variables with the liquid CO_2 at the ‘Product’ stream, by which the following results were obtained:

Table 27: Results of sensitivity analysis

Compressor 1 - Power Required (HP)	Compressor 2 - Power Required (HP)	Product - Mass Flow (Liquid 1) / Carbon dioxide (kg/s)
90000	200	14.8964
90000	225	14.8964
90000	250	14.8964
90000	275	14.8964
90000	300	14.8964
97500	200	14.8964
97500	225	14.8964
97500	250	14.8964
97500	275	14.8964
97500	300	14.8964
105000	200	14.8964
105000	225	14.8964
105000	250	14.8964
105000	275	14.8964
105000	300	14.8964
112500	200	14.8964
112500	225	14.8964
112500	250	14.8964
112500	275	14.8964
112500	300	14.8964
120000	200	14.8964
120000	225	14.8964
120000	250	14.8964
120000	275	14.8964
120000	300	14.8964

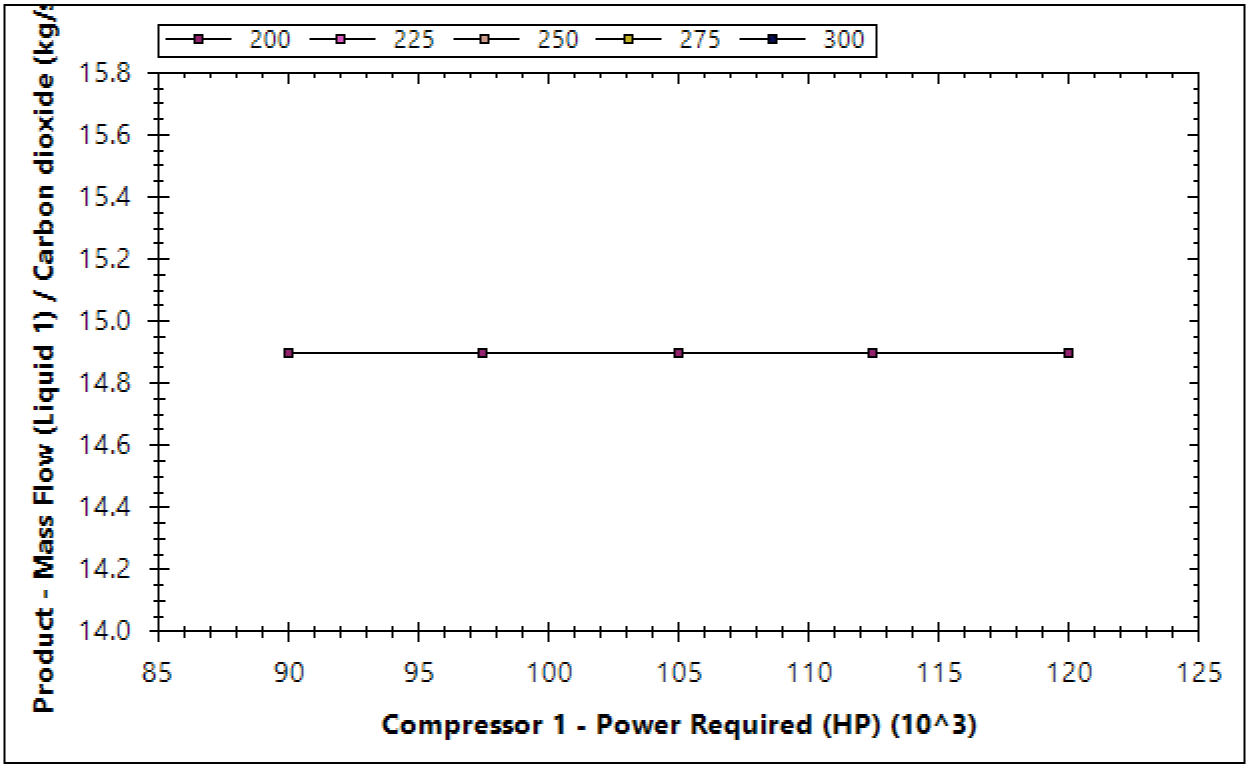


Figure 29: Graph vs. Compressor 1's power required and Compressor 2's power required vs. the flow rate of liquid CO_2

Similarly, the outlet temperatures of two coolers, 'cooler' and 'CL-2', were varied as independent variables, with the dependent variable being the 'Product' stream's outlet temperature. The following results were obtained for such a variation:

Table 28: Results of sensitivity analysis

cooler - Outlet Temperature (°C)	CL-2 - Outlet Temperature (°C)	Product - Mass Flow (Liquid 1) / Carbon dioxide (kg/s)
0	-100	13.745
0	-150	13.745
0	-200	13.745
0	-250	13.745

0	-300	13.745
-50	-100	13.8631
-50	-150	13.8631
-50	-200	13.8631
-50	-250	13.8631
-50	-300	13.8631
-100	-100	14.8964
-100	-150	14.8964
-100	-200	14.8964
-100	-250	14.8964
-100	-300	14.8964
-150	-100	15.18
-150	-150	15.18
-150	-200	15.18
-150	-250	15.18
-150	-300	15.18

The following graph was obtained for the above data in the Table 27:

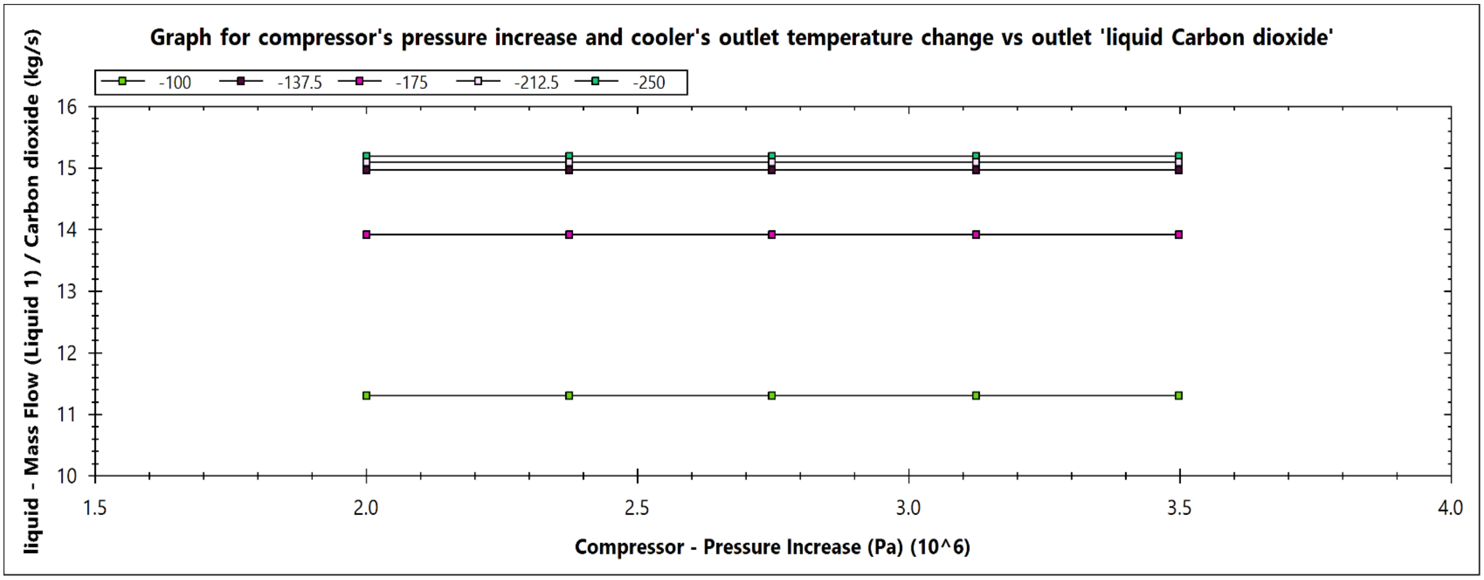


Figure 30: Graph for Compressor's pressure increase and cooler's outlet temperature vs outlet 'liquid CO_2

The above graph shows that there is a very low effect of change in coolers' temperature in our proposed model consisting of two stages.

Keeping the individual items in the same percentage displayed by graphs in Figure 20 and Figure 21, the DWSIM capital cost estimator for the year 2023 was used, setting the location as India to calculate the CAPEX, which is equal to $91,762,163.10, and the OPEX was found to be $40,107,879.66/year for various items, including the cost of ammonia feed and items like:

Fixed Costs:

- Maintenance costs
- Operation
- Laboratory
- Supervision
- Plant overheads
- Capital charges
- Rates/Taxes
- Insurance
- Licensing fees/ Royalty payments

Variable costs:

- Raw materials
- Other materials

Miscellaneous costs:

- Utilities
- Shipping and packaging

Since the cost in Nepal would be quite higher for every item discussed above than in India, influenced by factors such as transportation fees and shipping charges, the CAPEX was found to be approximately 92 million USD and the OPEX was found to be 41 million USD/year.

5.3.3. Three-stage compression system

In order to capture CO_2 completely in the liquid phase, 1 kg/s of ammonia was used in the feed for the only heat exchanger that acts as a cooler for the stream. The same amount of composition for feed was used as shown in Table 12 through Stream 2. Ammonia is sent on the shell side, and raw gas is sent on the tube side. The inlet conditions for the ammonia and design variables are taken from the available industrial data of flue gas.

The PR (Peng-Robinson) property package was used for all components. Vapor-liquid separators (like Separator-1) are used after the raw gas cooler to separate the liquid in the stream before compression. Five adiabatic compressors with an efficiency of 75% are used before the two flash columns. Five coolers with an efficiency of 100% are used after the flash columns.

In the first flash column, water and methanol are removed from the liquid stream, while carbon dioxide is recovered with other components in the vapor stream. In the second flash column, carbon dioxide is recovered in the liquid stream along with other components of flue gas, but in very low quantity compared to feed, as shown in the figure below:

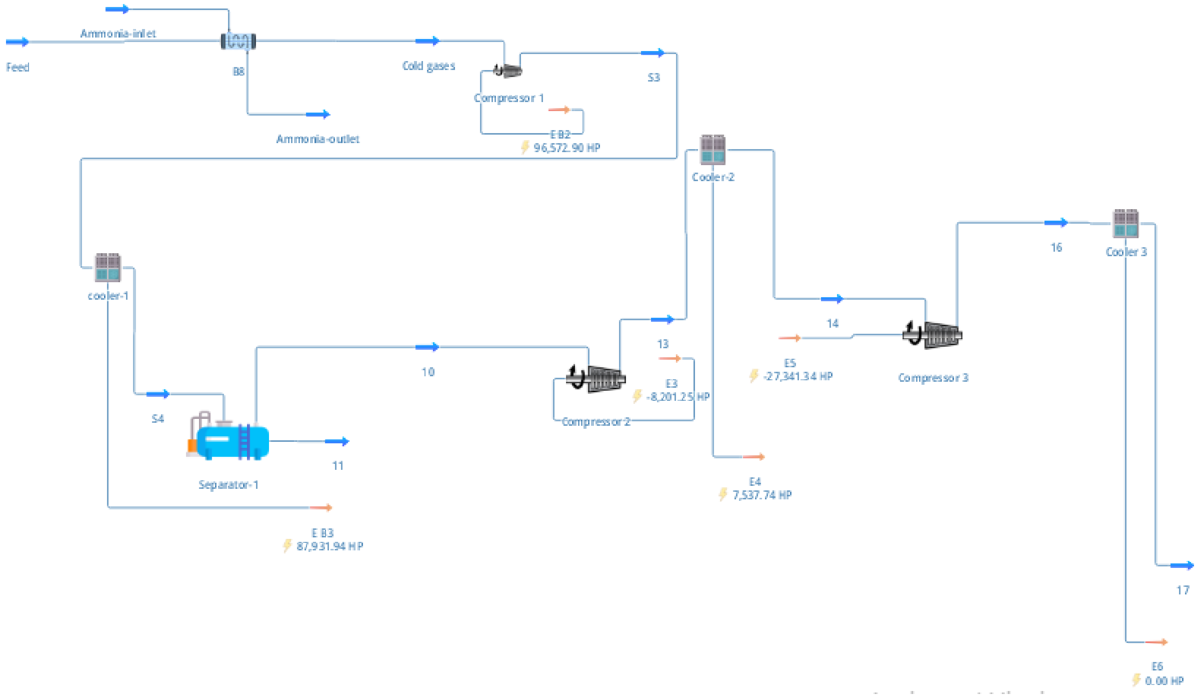


Figure 31: 3-stage compression and cooling

Following conditions were applied and output were generated on the stream used for different purposes each:

Table 29: Mass and energy balance at equipment

Name	**Mass Flow (kg/s)**	**Temperature (°C)**	**Pressure (bar)**	**Energy Flow (HP)**
17	100.007	-185.018	1	-222964
16	100.007	-185.018	1	-222964
14	100.007	-39.6657	30	-195623

13	100.007	10.6133	30	-188085
Ammonia-inlet	1	-3.5	3.77	-5542.61
11	0	51.3861	50	0
10	100.007	70.9557	50	-179884
S4	100.007	70.9557	50	-179884
S3	100.007	652.494	50	-91951.6
Cold gases	100.007	-3	0.997137	-188524
Feed	100.007	291.85	1	-146971
Ammonia-outlet	1	291.85	3.67	-2823.64

Table 30: Mass and energy balance at streams

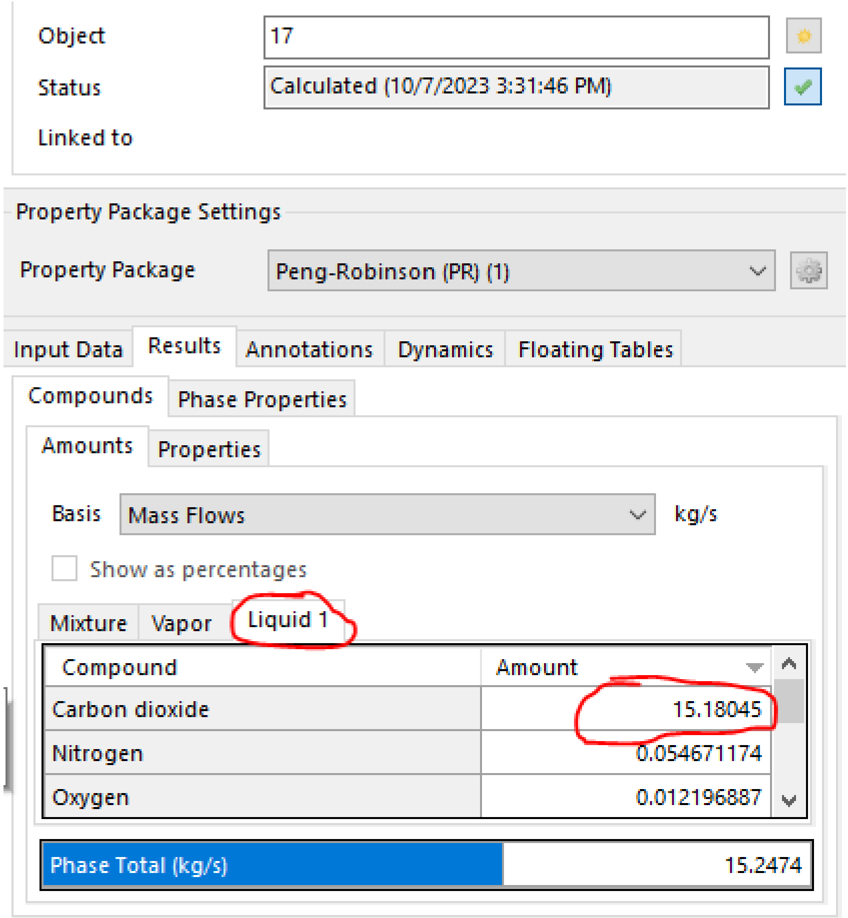
Name	**Mass Flow (kg/s)**	**Temperature (°C)**	**Pressure (bar)**	**Energy Flow (HP)**
17	100.007	-185.018	1	-222964
16	100.007	-185.018	1	-222964
14	100.007	-39.6657	30	-195623
13	100.007	10.6133	30	-188085
Ammonia-inlet	1	-3.5	3.77	-5542.61
11	0	51.3861	50	0
10	100.007	70.9557	50	-179884
S4	100.007	70.9557	50	-179884
S3	100.007	652.494	50	-91951.6
Cold gases	100.007	-3	0.997137	-188524

Feed	100.007	291.85	1	-146971
Ammonia-outlet	1	291.85	3.67	-2823.64

The ‘Feed’ stream was used for feeding the flue gas, consisting of the component gases with the same compositions as in Table 12. The following results were obtained in the final stream as liquid content:

Table 31: Mass flow rate of final stream’s components

Carbon dioxide	15.18045
Water	7.9503144E-05
Oxygen	0.012196887
Hydrogen	2.7649499E-08
Nitrogen	0.054671174
Ammonia	0
Carbon monoxide	1.1481054E-05



Object: 17

Status: Calculated (10/7/2023 3:31:46 PM)

Linked to

Property Package Settings

Property Package: Peng-Robinson (PR) (1)

Basis: Mass Flows kg/s

☐ Show as percentages

Compound	Amount
Carbon dioxide	15.18045
Nitrogen	0.054671174
Oxygen	0.012196887

Phase Total (kg/s): 15.2474

Figure 32: Final stream's CO_2 composition in the liquid phase

The sensitivity analysis was performed by varying the input ammonia mass flow rate at the 'Ammonia-inlet' stream, whereas the mass flow rate of the different components, including the carbon dioxide, was varied at the inlet stream 'Feed' so that the change in the mass flow rate of the product liquid CO_2 was determined at the 'Product' stream, as shown by Table 31 and the graph in Figure 33 below:

Table 32: Results of sensitivity analysis

Feed - Mass Flow (kg/s)	**Ammonia-inlet - Mass Flow (kg/s)**	**Product - Mass Flow (Liquid 1) / Carbon dioxide (kg/s)**
50	0	7.44771

50	1.25	7.44771
50	2.5	7.44771
50	3.75	7.44771
50	5	7.44771
75	0	11.1716
75	1.25	11.1716
75	2.5	11.1716
75	3.75	11.1716
75	5	11.1716
100	0	14.8954
100	1.25	14.8954
100	2.5	14.8954
100	3.75	14.8954
100	5	14.8954
125	0	18.6193
125	1.25	18.6193
125	2.5	18.6193
125	3.75	18.6193
125	5	18.6193
150	0	22.3431
150	1.25	22.3431
150	2.5	22.3431
150	3.75	22.3431
150	5	22.3431

The sensitivity analysis was performed for the model in Figure 31 for the variation of dependent variables with the independent variables:

Table 33: Results of sensitivity analysis

Feed - Mass Flow (kg/s)	**Ammonia-inlet - Mass Flow (kg/s)**	**17 - Mass Flow (Liquid 1) / Carbon dioxide (kg/s)**
50	0	7.58973
50	1.25	7.58973
50	2.5	7.58973
50	3.75	7.58973
50	5	7.58973
75	0	11.3846
75	1.25	11.3846
75	2.5	11.3846
75	3.75	11.3846
75	5	11.3846

Feed - Mass Flow (kg/s)	Ammonia-inlet - Mass Flow (kg/s)	17 - Mass Flow (Liquid 1) / Carbon dioxide (kg/s)
100	0	15.1795
100	1.25	15.1795
100	2.5	15.1795
100	3.75	15.1795
100	5	15.1795
125	0	18.9743
125	1.25	18.9743
125	2.5	18.9743
125	3.75	18.9743
125	5	18.9743
150	0	22.7692
150	1.25	22.7692
150	2.5	22.7692
150	3.75	22.7692
150	5	22.7692

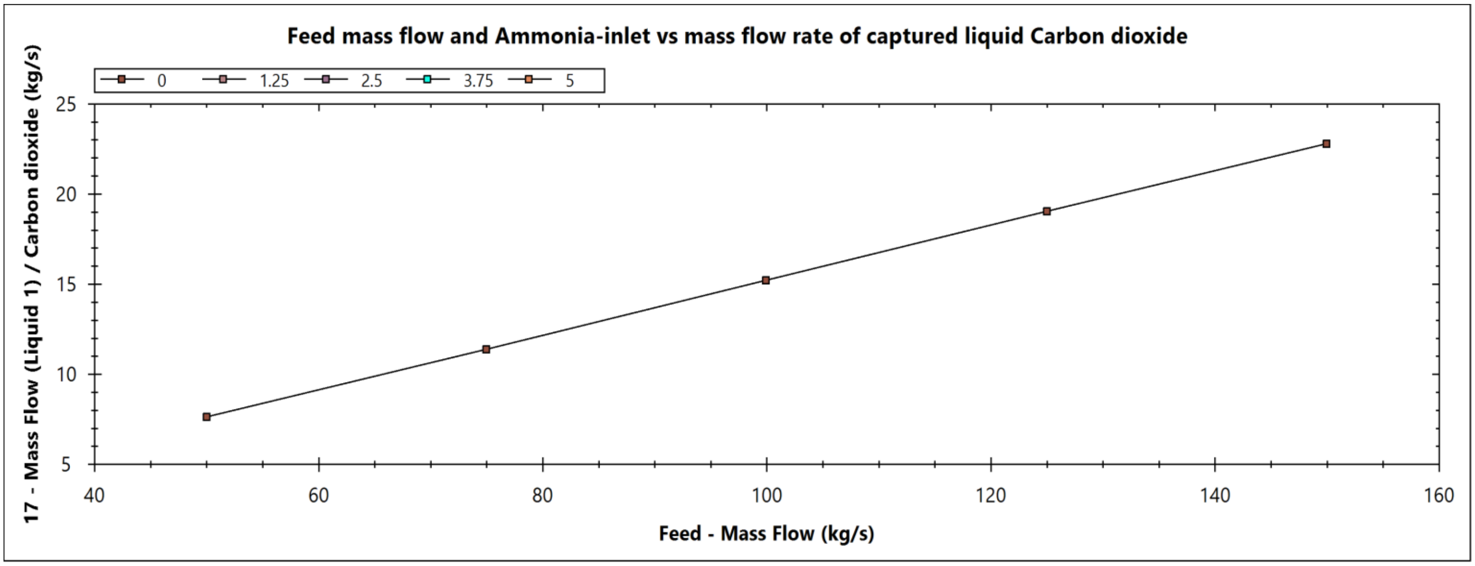


Figure 33: Plot for feed mass flow and ammonia-inlet vs captured liquid CO_2's flow rate

The above analysis shows that the feed flow rate at the 'Ammonia Inlet' does not have any impact on the capture of liquid CO_2, but the mass flow rate of flue gas with varying composition causes variation in the amount of liquid CO_2 captured.

Table 34: Table for sensitivity analysis

Feed - Mass Flow (kg/s)	**Ammonia-outlet - Temperature (°C)**	**17 - Mass Flow (Overall Liquid) / Carbon dioxide (kg/s)**
50	250	7.58973
50	275	7.58973
50	300	7.58973
50	325	7.58973
50	350	7.58973
75	250	11.3846
75	275	11.3846
75	300	11.3846
75	325	11.3846
75	350	11.3846
100	250	15.1795
100	275	15.1795
100	300	15.1795
100	325	15.1795
100	350	15.1795
125	250	18.9743
125	275	18.9743
125	300	18.9743
125	325	18.9743
125	350	18.9743
150	250	22.7692
150	275	22.7692
150	300	22.7692
150	325	22.7692
150	350	22.7692

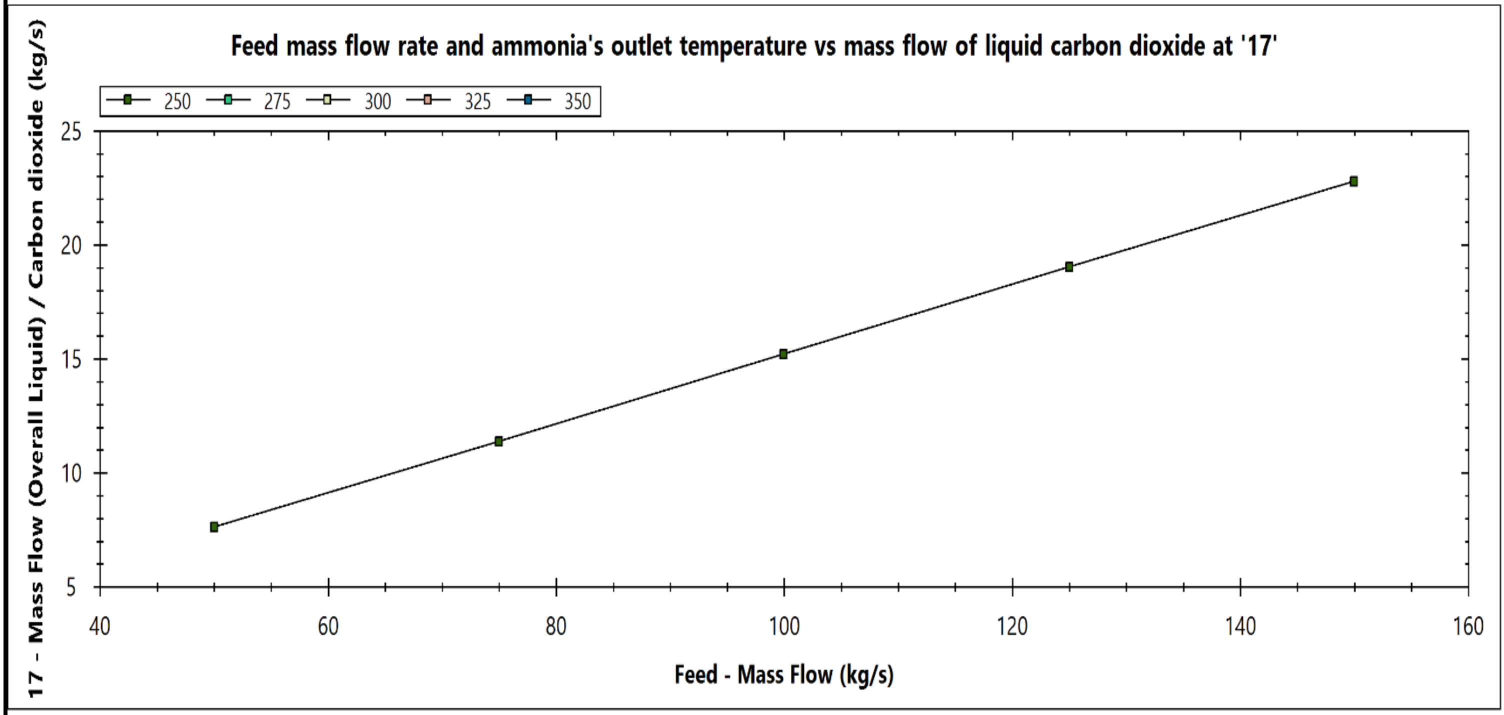


Figure 34: Plot for feed mass flow and ammonia's outlet temperature vs liquid CO_2 produced

The above table and analysis show the outlet liquid CO_2 concentration at the final stream '17' is independent of the ammonia's temperature at the outlet of the heat exchanger but is dependent on the flue gas composition at the 'Feed'.

The above table and analysis show the outlet liquid CO_2 concentration at the final stream '17' is independent of the ammonia's temperature at the outlet of the heat exchanger but is dependent on the flue gas composition at the 'Feed'.

Table 35: Results of sensitivity analysis

Feed - Mass Flow (kg/s)	**Compressor 1 - Power Required (HP)**	**17 - Mass Flow (Overall Liquid) / Carbon dioxide (kg/s)**
50	80000	7.58973
50	90000	7.58973
50	100000	7.58973
50	110000	7.58973
50	120000	7.58973
75	80000	11.3846
75	90000	11.3846
75	100000	11.3846
75	110000	11.3846
75	120000	11.3846

Feed - Mass Flow (kg/s)	**Compressor 1 - Power Required (HP)**	**17 - Mass Flow (Overall Liquid) / Carbon dioxide (kg/s)**
100	80000	15.1795
100	90000	15.1795
100	100000	15.1795
100	110000	15.1795
100	120000	15.1795
125	80000	18.9743
125	90000	18.9743
125	100000	18.9743
125	110000	18.9743
125	120000	18.9743
150	80000	22.7692
150	90000	22.7692
150	100000	22.7692
150	110000	22.7692
150	120000	22.7692

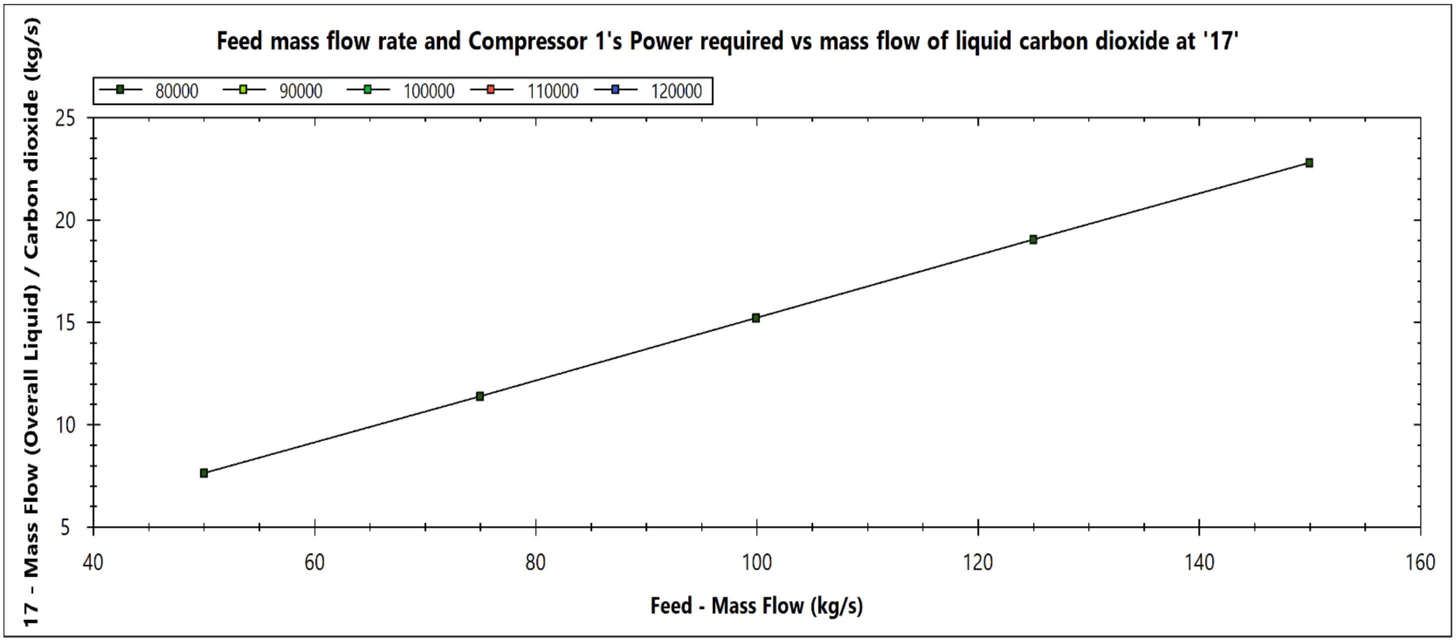


Figure 35: Variation of liquid CO_2 with mass flow of feed

Similarly, the power required for compressor 1 and the heat removed from cooler 1 were varied to determine the change in the overall mass flow of CO_2. The following results were obtained for such a variation:

Table 36: Results of sensitivity analysis

Compressor 1 - Power Required (HP)	**cooler-1 - Heat Removed (HP)**	**17 - Mass Flow (Overall Liquid) / Carbon dioxide (kg/s)**
80000	70000	15.1805
80000	75000	15.1805
80000	80000	15.1805
80000	85000	15.1805
80000	90000	15.1805
60037.5	70000	15.1805
60037.5	75000	15.1805
60037.5	80000	15.1805
60037.5	85000	15.1805
60037.5	90000	15.1805
40075	70000	15.1805
40075	75000	15.1805
40075	80000	15.1805
40075	85000	15.1805
40075	90000	15.1805
20112.5	70000	15.1805
20112.5	75000	15.1805
20112.5	80000	15.1805
20112.5	85000	15.1805
20112.5	90000	15.1805
150	70000	15.1805
150	75000	15.1805
150	80000	15.1805
150	85000	15.1805
150	90000	15.1805

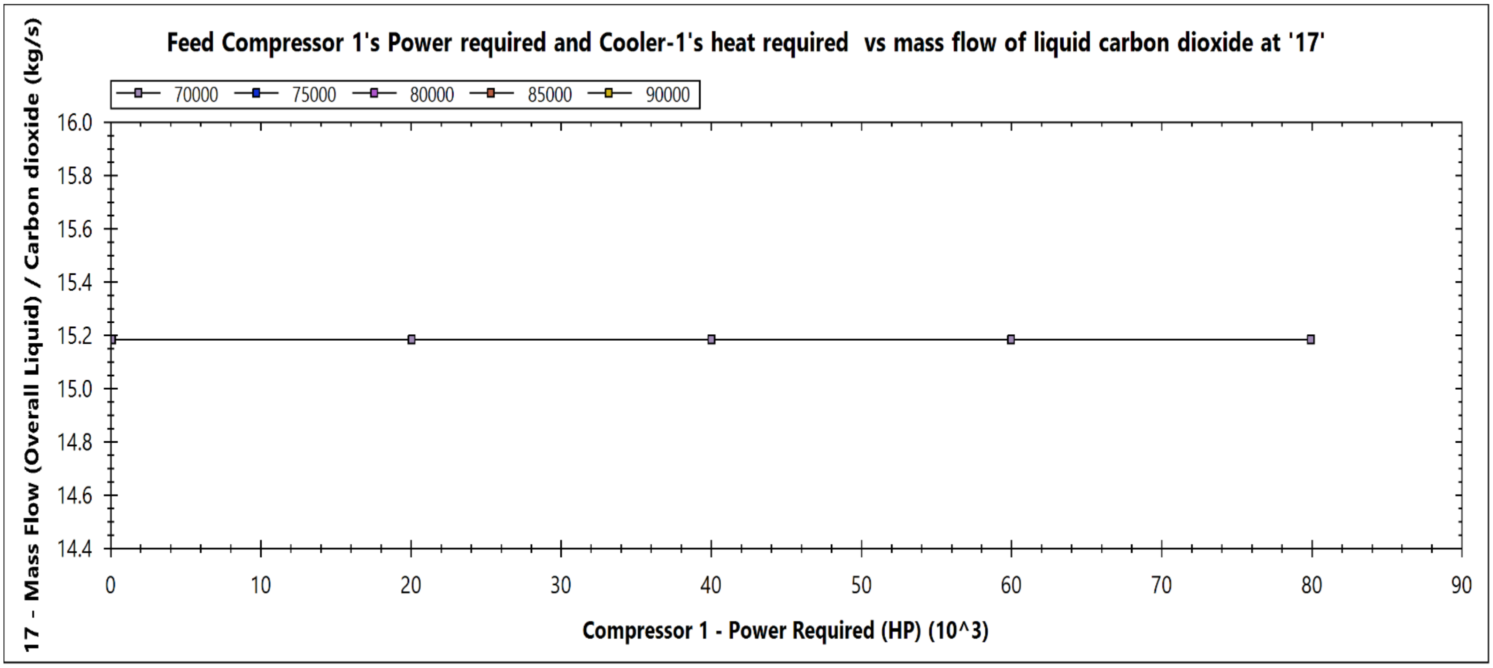


Figure 36: Feed Compressor 1's power required and Cooler 1's heat required vs mass flow of liquid CO_2

The above analysis shows that there is no effect on liquid carbon dioxide's mass flow rate at outlet '17' stream with the variation of compressor 1's power required and cooler 1's heat removed.

Similarly, the values of compressor 2's power required and cooler 2's heat removed were varied to determine the effect on liquid carbon dioxide's mass flow rate at outlet '17' stream, as shown below:

Table 37: Sensitivity study's results

Compressor 2 - Power Required (HP)	Cooler-2 - Heat Removed (HP)	17 - Mass Flow (Overall Liquid) / Carbon dioxide (kg/s)
-7000	6000	15.1805
-7000	27000	15.1805
-7000	48000	15.1805
-7000	69000	15.1805
-7000	90000	15.1805
-7500	6000	15.1805
-7500	27000	15.1805

Compressor 2 - Power Required (HP)	Cooler-2 - Heat Removed (HP)	17 - Mass Flow (Overall Liquid) / Carbon dioxide (kg/s)
-7500	48000	15.1805
-7500	69000	15.1805
-7500	90000	15.1805
-8000	6000	15.1805
-8000	27000	15.1805
-8000	48000	15.1805
-8000	69000	15.1805
-8000	90000	15.1805
-8500	6000	15.1805
-8500	27000	15.1805
-8500	48000	15.1805
-8500	69000	15.1805
-8500	90000	15.1805
-9000	6000	15.1805
-9000	27000	15.1805
-9000	48000	15.1805
-9000	69000	15.1805
-9000	90000	15.1805

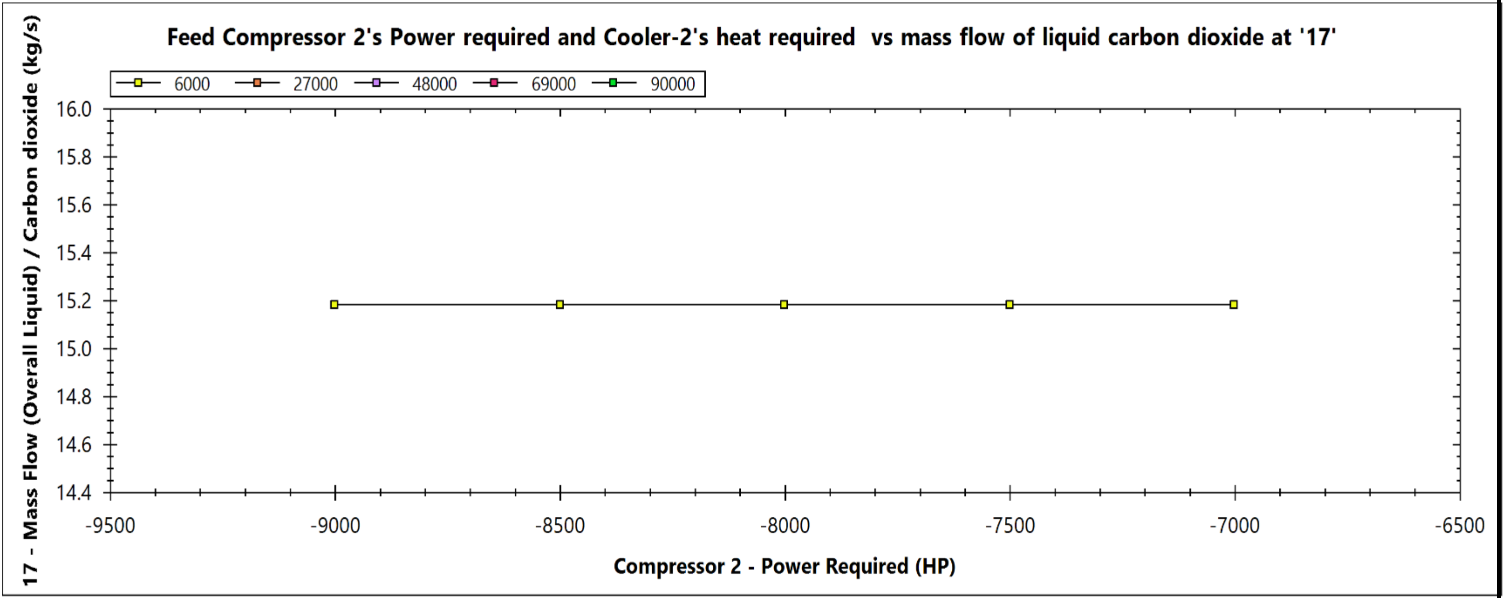


Figure 37: Feed compressor 2's power required and cooler 2's heat required vs mass flow rate of liquid CO_2

The above results show that there is no effect on outlet liquid CO_2 by the variation of compressor 2's power required and cooler 2's outlet temperature.

Similarly, the power required for compressor 3 and the outlet temperature of cooler 3 were varied as independent variables to see the effect on liquid composition on outlet stream '17'.

Table 38: Results of sensitivity analysis

Compressor 3 - Power Required (HP)	Cooler 3 - Outlet Temperature (°C)	17 - Mass Flow (Overall Liquid) / Carbon dioxide (kg/s)
-260000	-100	15.1805
-260000	-150	15.1805
-260000	-200	15.1805
-260000	-250	15.1805
-260000	-300	15.1805
-267500	-100	15.1805
-267500	-150	15.1805
-267500	-200	15.1805
-267500	-250	15.1805
-267500	-300	15.1805
-275000	-100	15.1805
-275000	-150	15.1805
-275000	-200	15.1805

Compressor 3 - Power Required (HP)	Cooler 3 - Outlet Temperature (°C)	17 - Mass Flow (Overall Liquid) / Carbon dioxide (kg/s)
-275000	-250	15.1805
-275000	-300	15.1805
-282500	-100	15.1805
-282500	-150	15.1805
-282500	-200	15.1805
-282500	-250	15.1805
-282500	-300	15.1805
-290000	-100	15.1805
-290000	-150	15.1805
-290000	-200	15.1805
-290000	-250	15.1805
-290000	-300	15.1805

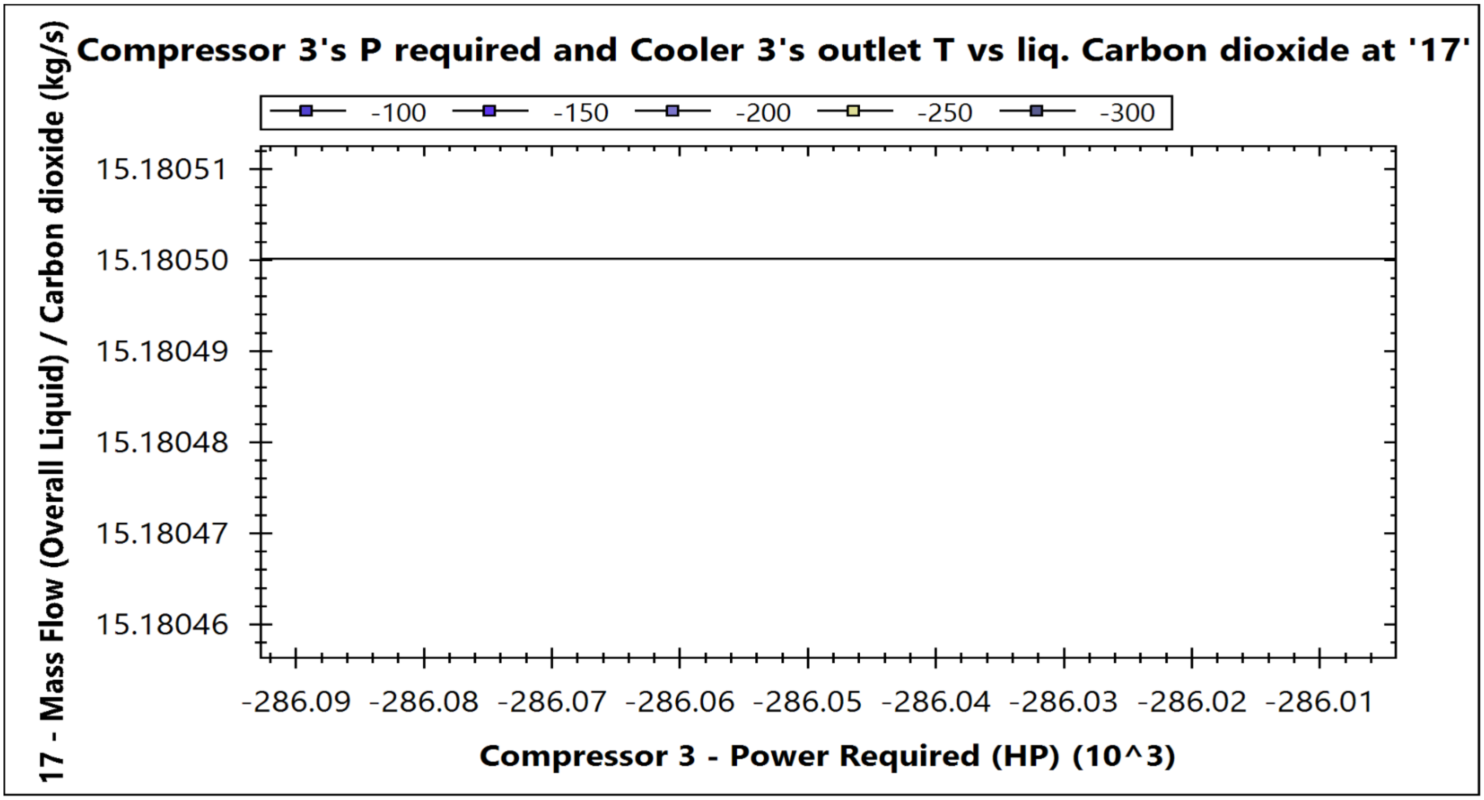


Figure 38: Compressor 3’s power (P) required and cooler 3’s outlet temperature vs liquid CO_2

The above analysis shows that a small change in compressor 3’s power required and cooler 3’s outlet temperature has no effect on the mass flow rate of liquid CO_2 at outlet stream ‘17’.

Similarly, compressor 1's power required and cooler 2's outlet temperature were varied to check the effect on liquid CO_2 produced on stream '17', by which the following results were obtained:

Table 39: Results of sensitivity study

Compressor 1 - Power Required (HP)	**Cooler-2 - Outlet Temperature (°C)**	**17 - Mass Flow (Overall Liquid) / Carbon dioxide (kg/s)**
90000	-20	15.1805
90000	-25	15.1805
90000	-30	15.1805
90000	-35	15.1805
90000	-40	15.1805
92500	-20	15.1805
92500	-25	15.1805
92500	-30	15.1805
92500	-35	15.1805
92500	-40	15.1805
95000	-20	15.1805
95000	-25	15.1805
95000	-30	15.1805
95000	-35	15.1805
95000	-40	15.1805
97500	-20	15.1805
97500	-25	15.1805
97500	-30	15.1805
97500	-35	15.1805
97500	-40	15.1805
100000	-20	15.1805
100000	-25	15.1805
100000	-30	15.1805
100000	-35	15.1805
100000	-40	15.1805

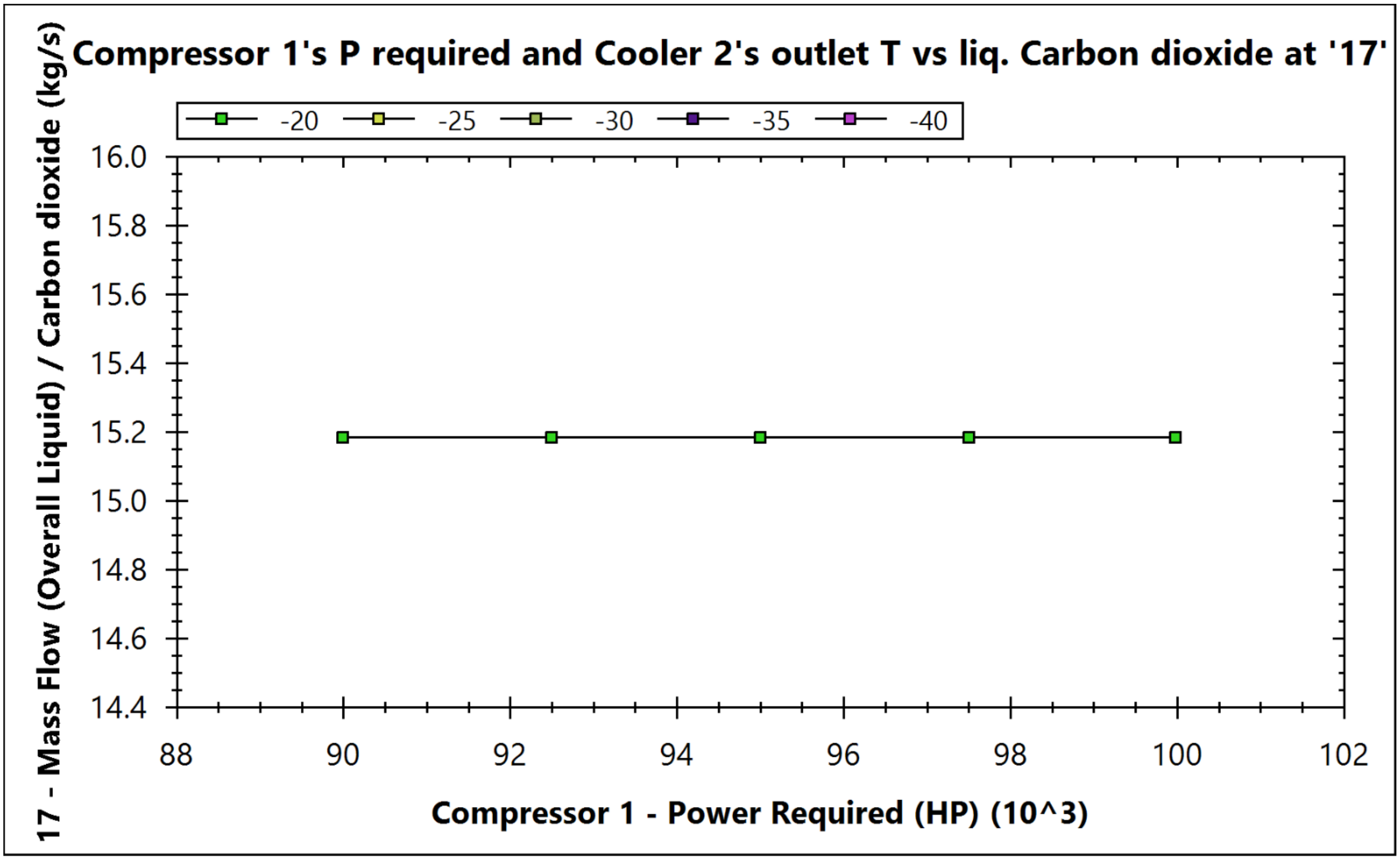


Figure 39: Compressor 1’s power (P) required vs cooler 2’s outlet temperature vs liquid CO_2

The above results show that there is no effect on outlet liquid CO_2 production at the outlet stream with the variation in compressor 1’s power required and cooler 2’s outlet temperature.

Similarly, compressor 2’s power required and cooler 3’s outlet temperature were varied to check the effect on liquid CO_2 produced on stream '17', by which the following results were obtained:

Table 40: Results of sensitivity analysis

Compressor 2 - Power Required (HP)	Cooler 3 - Heat Removed (HP)	17 - Mass Flow (Overall Liquid) / Carbon dioxide (kg/s)
19375	20	15.1805
46250	-20	15.1804
46250	-10	15.1804
46250	0	15.1805
46250	10	15.1805
46250	20	15.1805
73125	-20	15.1804
73125	-10	15.1804
73125	0	15.1805

Compressor 2 - Power Required (HP)	Cooler 3 - Heat Removed (HP)	17 - Mass Flow (Overall Liquid) / Carbon dioxide (kg/s)
73125	10	15.1805
73125	20	15.1805
100000	-20	15.1804
100000	-10	15.1804
100000	0	15.1805
100000	10	15.1805
100000	20	15.1805

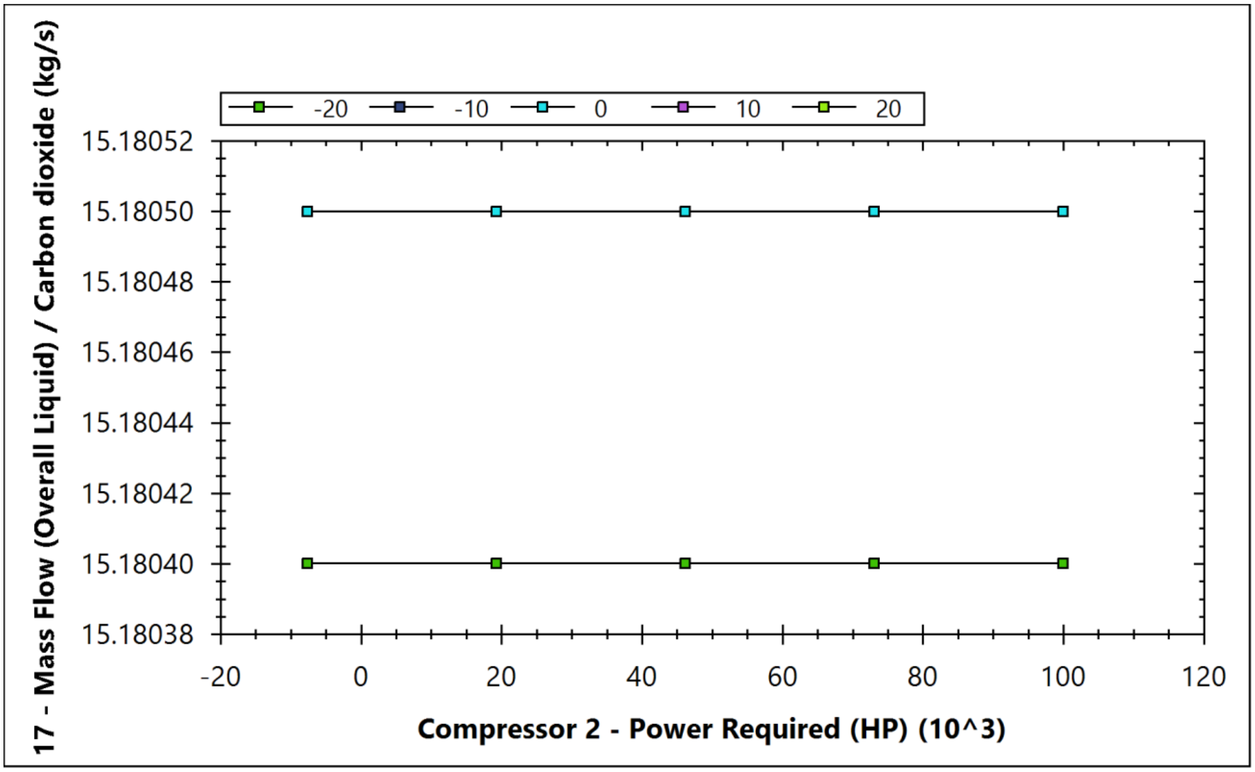


Figure 40: Compressor 2's power required and cooler 3's heat removed and mass flow of overall liquid CO_2

The above results show that there is a very low effect of a small change in compressor 2's power required and cooler 3's outlet temperature on liquid CO_2 produced on stream '17'.

Similarly, compressor 1's power required and cooler 3's outlet temperature are varied to check the effect on liquid CO_2 produced on stream '17', by which the following results were obtained:

Table 41: Results of sensitivity analysis

Compressor 1 - Power Required (HP)	**Cooler 3 - Heat Removed (HP)**	**17 - Mass Flow (Overall Liquid) / Carbon dioxide (kg/s)**
80000	-20	15.1804
80000	-10	15.1804
80000	0	15.1805
80000	10	15.1805
80000	20	15.1805
85000	-20	15.1804
85000	-10	15.1804
85000	0	15.1805
85000	10	15.1805
85000	20	15.1805
90000	-20	15.1804
90000	-10	15.1804
90000	0	15.1805
90000	10	15.1805
90000	20	15.1805
95000	-20	15.1804
95000	-10	15.1804
95000	0	15.1805
95000	10	15.1805
95000	20	15.1805
100000	-20	15.1804
100000	-10	15.1804
100000	0	15.1805
100000	10	15.1805
100000	20	15.1805

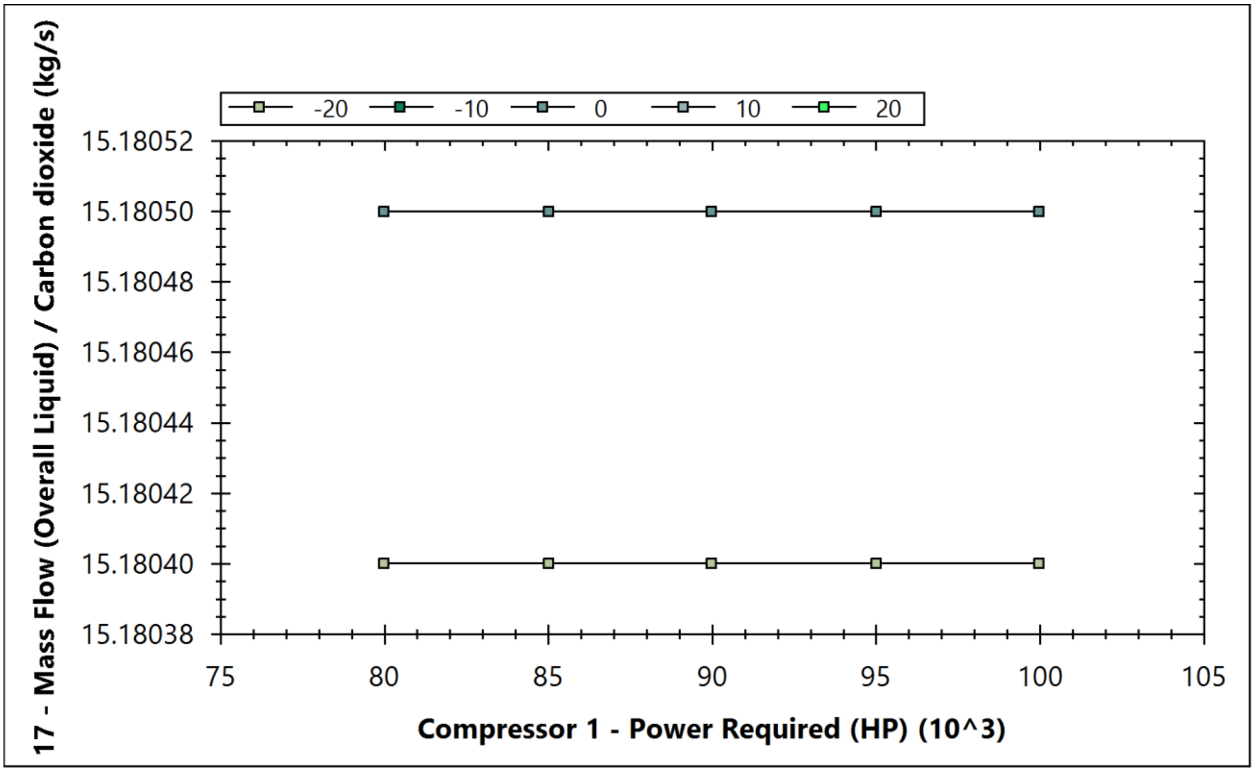


Figure 41: Compressor 1's power required and Cooler 3's heat removed vs mass flow of overall liquid CO_2

For this type of compression, a single gas-liquid separator was used to evaluate if the triple-stage compression method's cost could be reduced, but the CAPEX for the percentage of similar items as shown in Table 17 and the same percentage of individual items was found to be $148,527,990.03, and the total OPEX for the cost, including that of ammonia fed in the 'Ammonia-inlet' stream, was found to be $49,166,669,81/year, setting the base location as India. The CAPEX can be approximated to be 149 million USD and the OPEX 50 million USD/year since the price in Nepal would surely be higher for the establishment of such a plant that is influenced by factors like transportation, shipping charges, availability of raw materials, etc. The OPEX was calculated for the following items, including the cost of ammonia:

Fixed Costs:

- Maintenance costs
- Operation
- Laboratory
- Supervision
- Plant overheads
- Capital charges
- Rates/Taxes
- Insurance

- Licensing fees/ Royalty payments

Variable costs:

- Raw materials
- Other materials

Miscellaneous costs:

- Utilities
- Shipping and packaging

From the above overall analysis, we find that the cost of the CO_2 compression and cooling plant for the carbon capture plant for capturing the carbon dioxide being generated in the Shivam Cement Industry is very high, but if the carbon capture is done utilizing these processes for cryogenic CO_2 capture, then the problem of CO_2 emissions from this industry, which is one of the largest CO_2 emitters in Nepal, would be solved.

But from our analysis, the safer and cheaper process is found to be 2-stage compression, as shown by Figure 24. Since, for the single-stage process, the CAPEX is higher than 2nd, and for 3rd, the cost is higher than 2nd too. Similarly, OPEX is lowest in the case of two-stage compression, as shown by Table 40 below:

Table 42: CAPEX and OPEX/year

Model's number of stages	CAPEX	OPEX
1 (Figure 18)	$112,000,000	$56,000,000/year
2 (Figure 24)	$92,000,000	$41,000,000/year
3 (Figure 31)	$149,000,000	$50,000,000/year

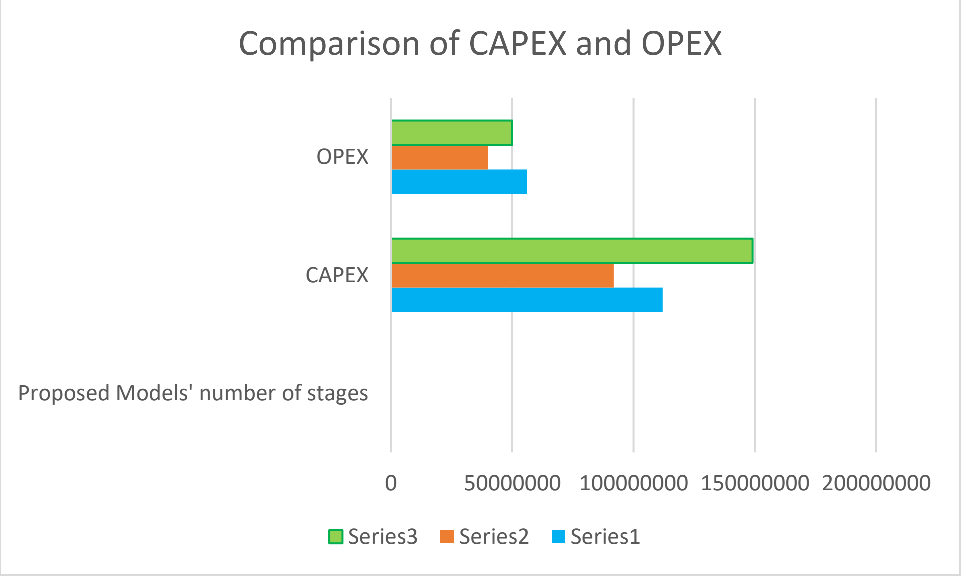


Figure 42: Comparison of CAPEX and OPEX for all three stage

Since the CAPEX for the second model we proposed, as shown in Figure 24, has a lower cost and is a two-stage cooling and compression process, our study finds that the second model we proposed for capturing flue gas can be applicable in the Sarbottam Cement Industry of Nepal.

The capital cost of building the two-stage compression and cooling model for CO_2 capture is found to be $92,000,000, and since the Nepali industry can purchase the CO_2 capture tank more easily from India than from other countries, the capital cost of a storage tank purchased for storing the captured liquid CO_2 would be around $33,041.96 for a tank of 5000 L capacity and a maximum design pressure of 15-20 bar [36].

When the cost of the 5000-liter tank discussed above and the cost of the two-stage compression model are summed up, the total cost of the carbon capture and storage plant is $92,033,041.96, which can be approximated to $92,050,000 as the cost of the storage tank would be higher in Nepal due to taxes on import and transportation costs.

Devkota et al., through their research [34], found their model to be capable of capturing 96.6 mol% CO_2. However, our proposed two-stage compression model is able to capture CO_2 of very high purity (99.30%), which is very close to the value of the purity of captured liquid CO_2 to form ammonia compared to the model described in [34], as shown below:

Table 43: Feed’s vs product’s purity

Compounds	Feed's mass flow rate (kg/s)	Product's mass flow rate (kg/s)	Feed's % purity	Product's % purity
Carbon dioxide	15.18	14.89641	15.18	99.30937
Water	7.95E-05	7.95E-05	7.95E-05	0.00053
Oxygen	0.652	0.006834	0.652	0.04556
Hydrogen	0.019	2.61E-06	0.019	1.74E-05
Nitrogen	84.14	0.053291	84.14	0.355271
Ammonia	0	0	0	0
Carbon monoxide	0.0155	1.09E-05	0.0155	7.29E-05

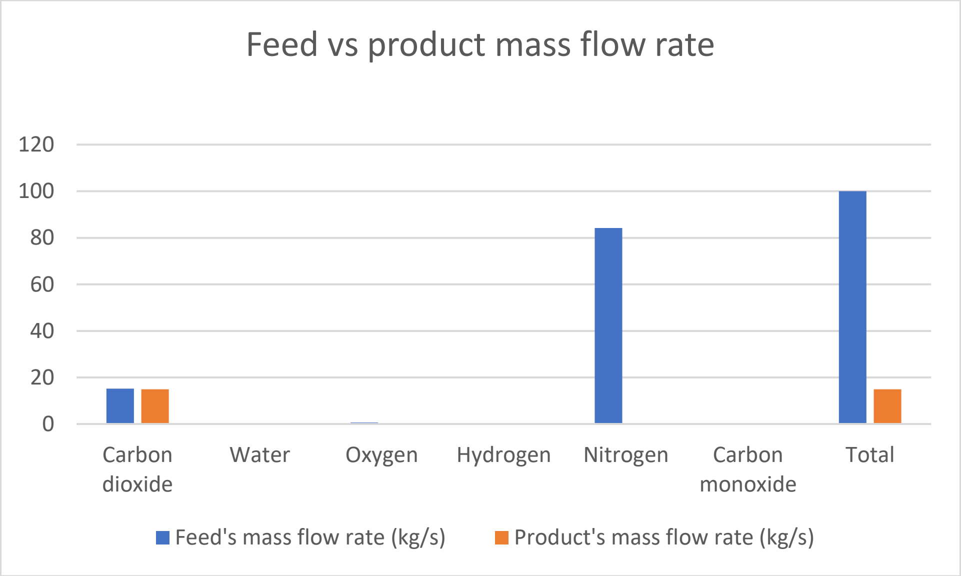


Figure 43: Feed’s vs product’s mass flow rate

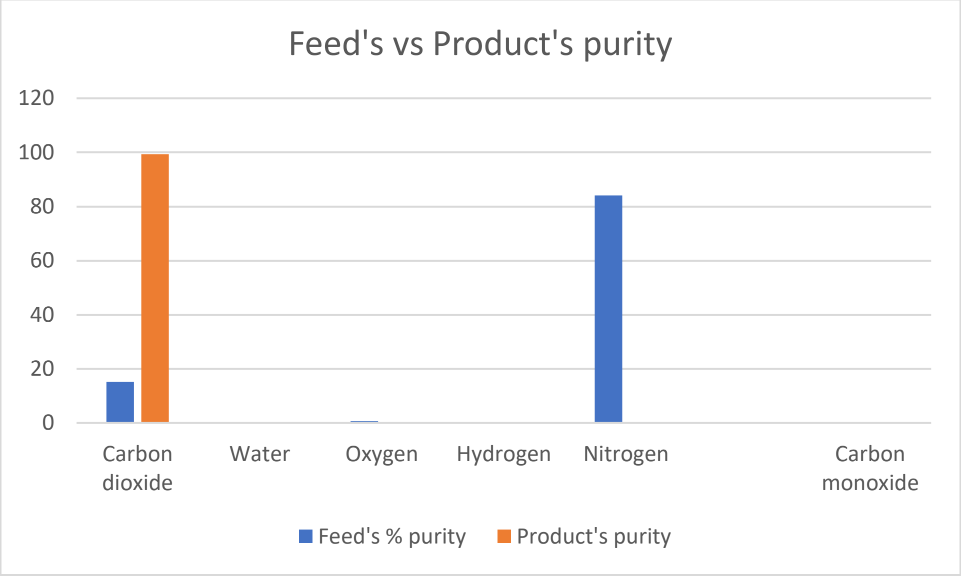


Figure 44: Feed’s vs product’s purity

The above results show that the proposed model of 2-stage compression and cooling is costly but can be useful to obtain CO_2 of very high purity that can be directly used to form urea and methane compounds without any further treatment of the captured liquid CO_2.

5.4. Economic evaluation

The various economical parameters are determined to find the profit/loss gained over the investment.

5.4.1. Levelized cost of CO_2 abatement (LCCA)

The levelized cost of CO_2 abatement (LCCA) is a measure of how much CO_2 can be reduced by a specific investment or policy, taking into account relevant factors related to geography and specific assets. It calculates how much an investment or policy costs on the basis of dollars per ton of emissions reduced. The output is always money per unit CO_2 equivalent reduction, or $/ton [37].

The levelized cost of carbon abatement (LCCA) is a tool that can help investors and policymakers assess the cost-effectiveness of different carbon reduction strategies. It measures how much CO_2 can be reduced by a specific investment or policy, taking into account relevant factors related to geography and specific assets. It calculates how much an investment or policy costs on the basis of dollars per ton of emissions reduced.

The formula for LCCA is as follows:

$$\text{LCCA} = \frac{Total\ cost\ of\ investment}{Total\ CO_2\ reduction} \qquad (1)$$

where:

The total cost of investment is the sum of all costs associated with the investment or policy, including capital, operating, and maintenance costs.

Total CO_2 reduction is the total amount of CO_2 that will be reduced by the investment or policy **Error! Reference source not found.**.

Then, if we assume a total of 20 years of project life, the plant generates CO_2 = project life × mass flow rate of CO_2 (kg/sec) × 86400 sec/year = 20 × 14.89641 × 86400 = 25740996.5 kg CO_2, which is equal to total CO_2 reduction. Since the CAPEX for our proposed 2-stage model is $92,000,000,

then LCCA = $\frac{CAPEX}{Total\ CO_2\ reduction}$ (2)

So, LCCA = $3.57/Kg CO_2

The electricity cost per kilowatt-hour (kWh) in Nepal is 5.79 Nepalese rupees (NPR) for households and 9.21 NPR for businesses as of the present date. According to Google Finance, the exchange rate on the present date is 1 NPR = 0.0076 USD. Therefore, the cost of electricity per kWh in USD is: For businesses: 9.21 NPR/kWh × 0.0076 USD/NPR = 0.069 USD/kWh.

The calculated CAPEX and OPEX are based on the standard procedures that the DWSIM software follows for capital cost estimation. The price of electricity is estimated to be 0.069$/kWh on the basis of tariffs that are set by the Nepal Electricity Authority (NEA). But the Nepali government had signed to provide a subsidy of $0.005 per kg of CO_2 captured, which was considered based on the Emission Reduction Purchase Agreement (ERPA) with the World Bank in February 2021.

Although the captured CO_2 is quite costly, it can help create a significant quantity of urea. The return on investment (ROI) and the payback period are calculated to analyze the profitability of the plant as a standalone plant.

5.4.2. Net Present Value

The net present value (NPV) is a financial metric used to evaluate the profitability of an investment or project. It represents the difference between the present value of cash inflows and outflows over a specified time period. The formula to calculate NPV is as follows:

$$\text{NPV} = \frac{\sum CF_t}{(1+r)^t} - C_0 \qquad (3)$$

where:

NPV = Net Present Value

$\sum$ = Summation symbol, meaning you need to calculate this for each period and sum the results.

CFt = Cash flow during a specific period 't'

r = Discount rate (the rate of return required to make the investment or project worthwhile)

t = Time period

C_0 = Initial investment (usually at time t=0)

If CFT = profit%/100 × CAPEX + CAPEX, profit=5%, CAPEX = $92,000,000, r=0.05 (5%), t = 2, 4, 6, 8, 10, 12, 14, 16, 18, 20 years and C_0 = CAPEX, plot for variation of NPV with number of years is given by:

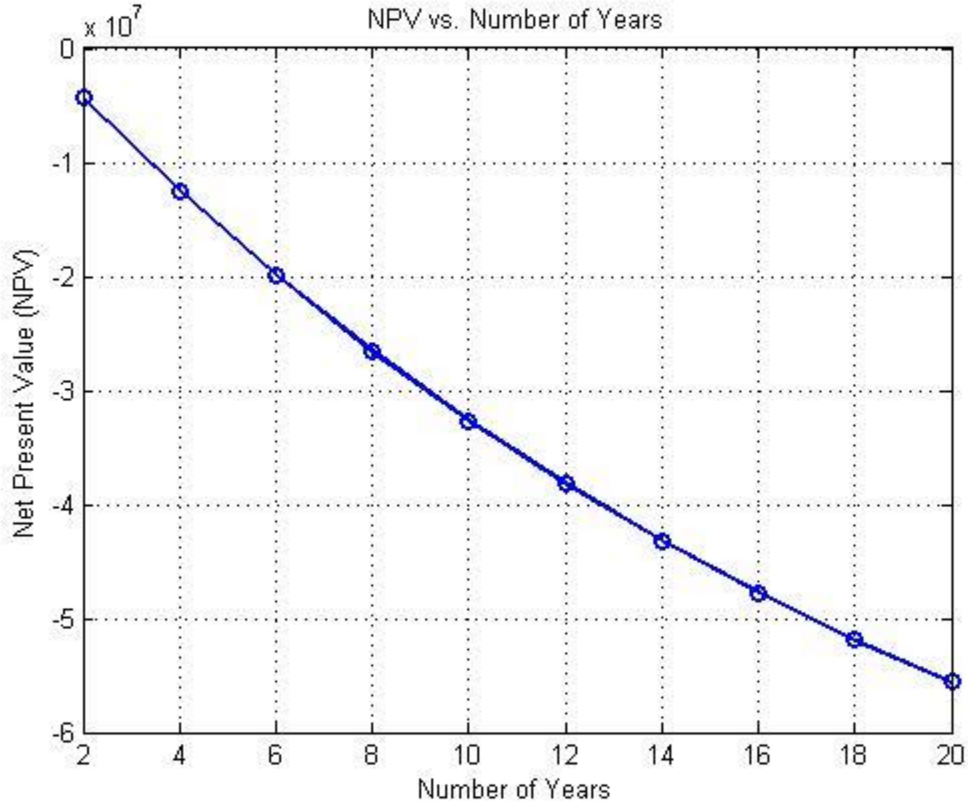


Figure 45: Plot for NPV vs number of years

if CFT = profit/100 × CAPEX + CAPEX, profit = 2, 4, 6, 8, 10, 12, 14, CAPEX = $92,000,000, r = 0.05, t = 5, 10, 15, 20 years and C_0 = CAPEX, then the plot for variation of NPV with profit for specific number of years is:

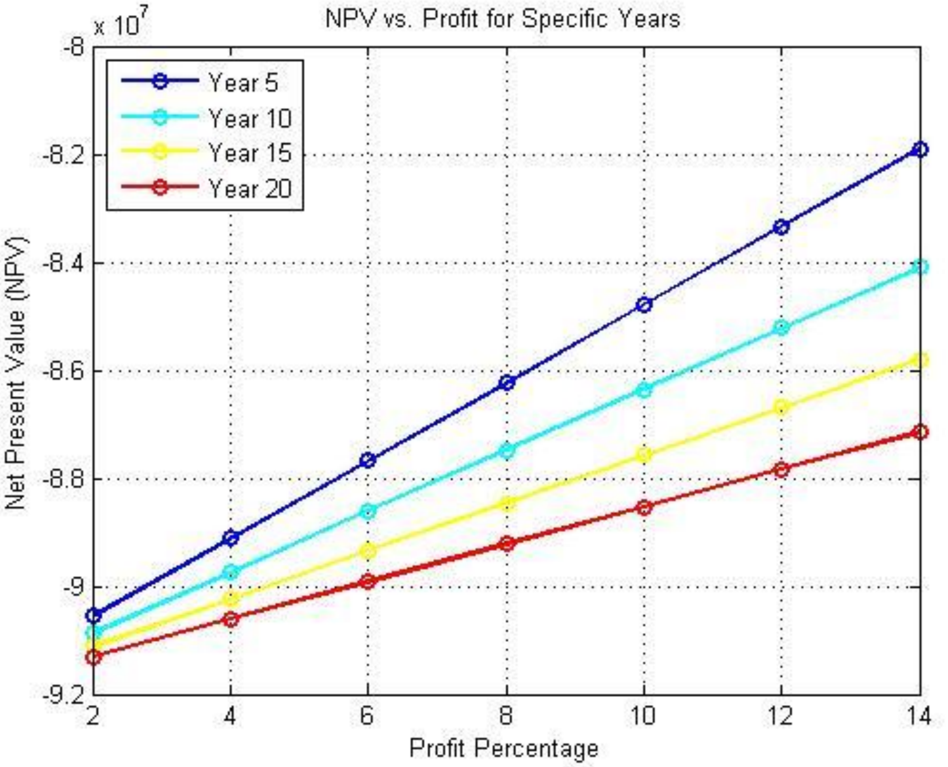


Figure 46: NPV vs profit percentage value plot

5.4.3. Return of Investment

Similarly, the Return of Investment (ROI) is given by:

$$\text{ROI} = \frac{Profit}{Cost\ of\ Investment} \times 100\% \qquad (4)$$

where:

ROI is Return on Investment, expressed as a percentage.

Net Profit: The total profit generated from the investment, which is usually calculated as the total gain minus the initial cost or investment.

Cost of Investment: The initial amount of money invested in the project or investment.

If net profit = 1%, 2%, 3%, 4%, 5%, 10%, 20%, 25% of Cost of Investment and Cost of Investment = $92,000,000, then the single plot for ROI values for different values of net profit is:

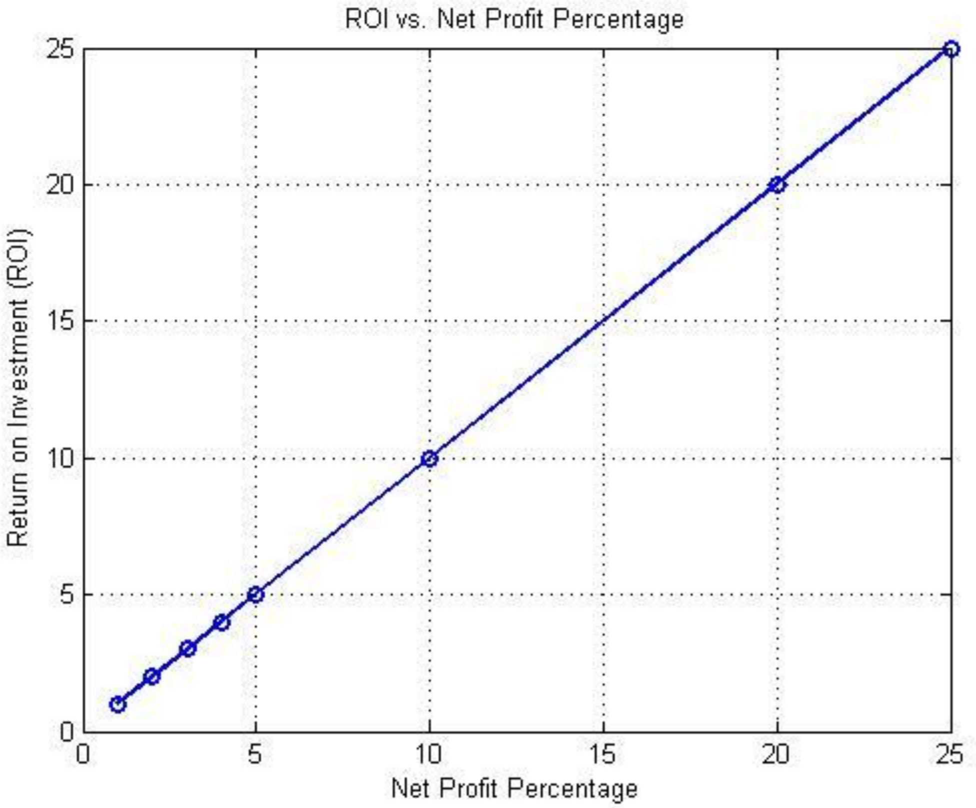


Figure 47: ROI vs NPV

if CFT = profit/100 × CAPEX, profit% = 2%, 4%, 6%, 8%, 10%, 12%, 14%, CAPEX = $92,000,000, r = 0.05, 0.1 ,0.15, 0.2, t = 5, 10, 15, 20 years and C_0 = CAPEX then the NPV varies with profit%, CAPEX and time period as shown by plot below:

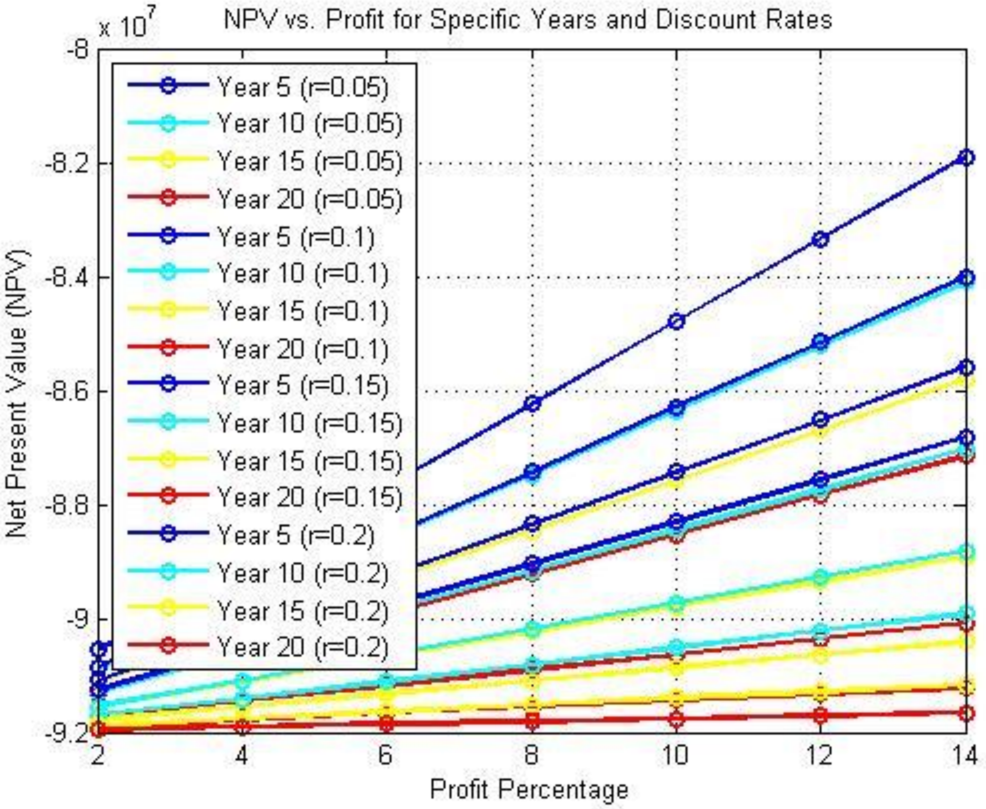


Figure 48: NPV vs profit percentage

5.4.4. Payback Period

Similarly, the Payback Period is calculated by:

$$\text{Payback Period} = \frac{Initial\ investment}{Annual\ cash\ flow} \qquad (5)$$

When the annual cash flow is assumed to be 0.5%, 1%, 1.5%, 2%, 2.5%, 3%, 3.5%, 4%, 4.5%, and 5% of the initial investment, then the payback period varies with the annual cash flow, as shown by the plot below:

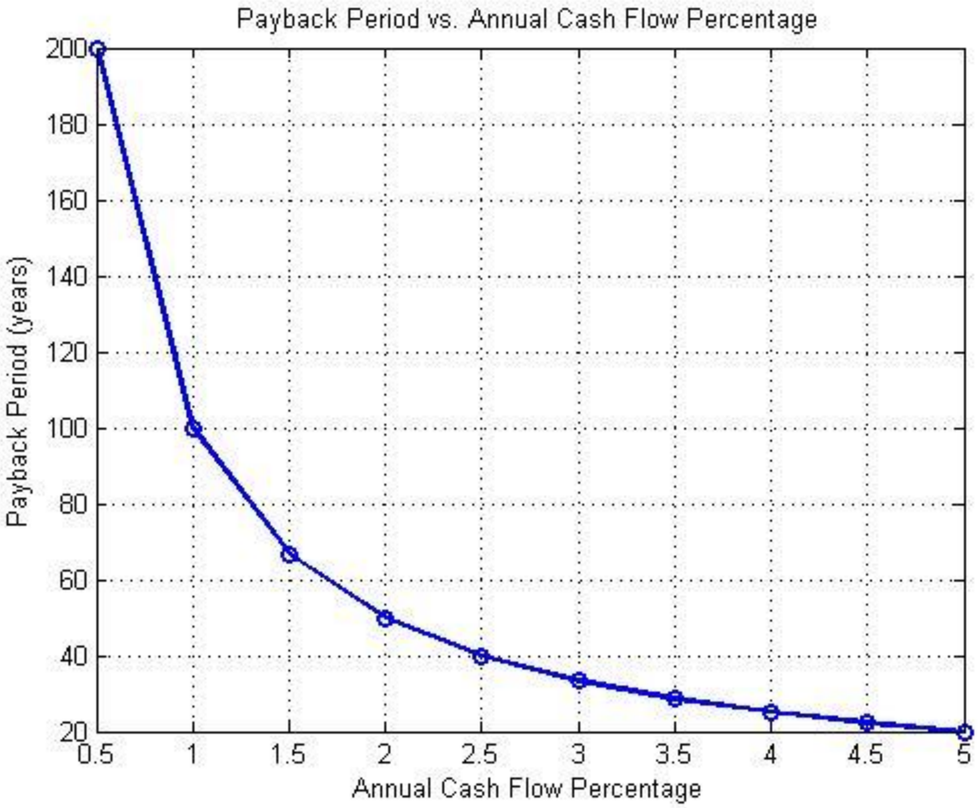


Figure 49: Payback period vs annual cash flow %

According to the report by [38], based on the average inflation rate in Nepal from 1965 to 2021, the average inflation rate in Nepal was 8.0% per year. Using the same average value of the inflation rate, assuming there is an effect on the OPEX value and a rise in the OPEX value per year, The effect on OPEX value per year is shown by the plot and Table 42 below for 20 years from the beginning year of the project in 2023:

Table 44: Rise in OPEX/year

Year	OPEX/year (millions USD)
1	41
2	43.68
3	46.53
4	49.61
5	52.9
6	56.41
7	60.12
8	64.02
9	68.1
10	72.36
11	76.8
12	81.44
13	86.26
14	91.28
15	96.51
16	102.03
17	107.77
18	113.73
19	119.91
20	126.31

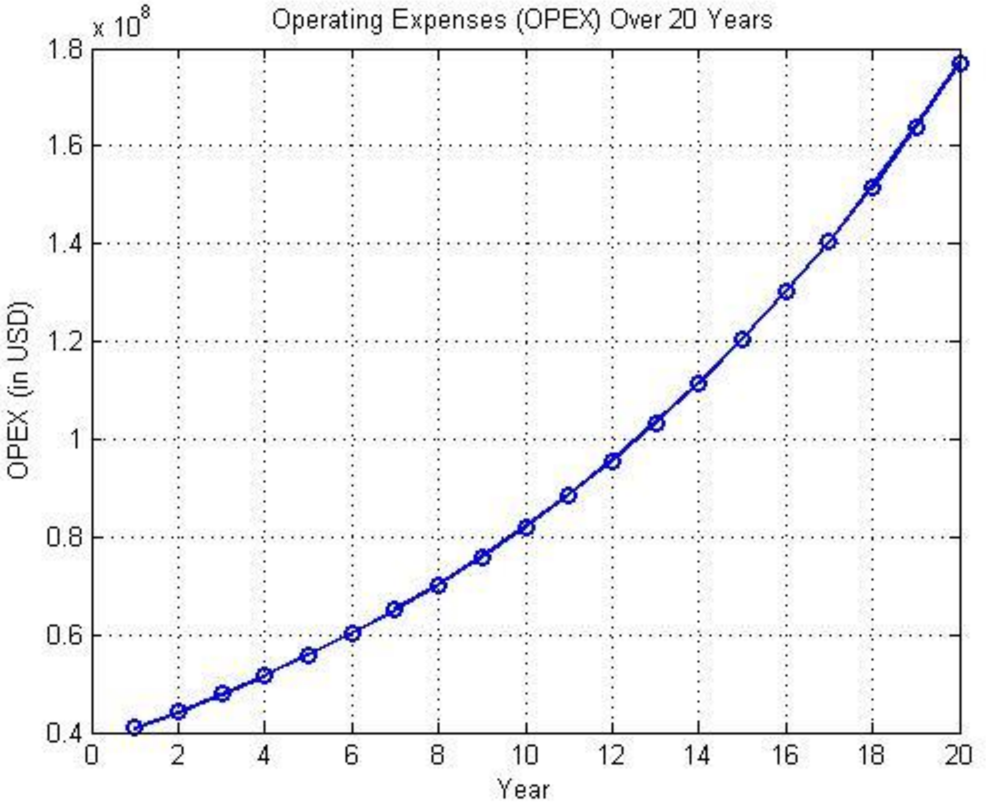


Figure 50: OPEX value rise per year

According to **Error! Reference source not found.**[29], customs duties are generally assessed on the cost, insurance, and freight (CIF) value. Imported goods are also liable for a value-added tax (VAT) of '13 percent' levied on CIF plus customs duty value. This VAT value mostly affects the CAPEX and OPEX in our overall estimation and economic analysis.

6. Applications of Cryogenic compression method

The membrane separation method is not completely effective for CO_2 capture. So, in order to obtain CO_2 in completely pure form or very close to 100% purity, cryogenic compression technology can be combined with the membrane separation method. We can take the example of the Rectisol Wash Process for the Removal of H_2S and CO_2 from Sour Syngas, where the quantity of CO_2 captured is very low, which can be increased by including the cooler and compressor for cryogenic CO_2 capture.

6.1. Rectisol Wash Process for Removal of H_2S and CO_2 from Sour Syngas

The rectisol wash process is a common process used in process industries, mainly for the Rectisol wash process is a method used for the purification and separation of gases, particularly carbon dioxide (CO_2) and hydrogen sulfide (H_2S), from gas streams in various industrial applications. This process utilizes a solvent to selectively capture and remove the impurities from the gas stream, which is actually a membrane separation method. Here are some common uses of the Rectisol wash process:

Natural Gas Purification: Rectisol is often employed to remove impurities such as CO_2, H_2S, and other sulfur compounds from natural gas streams, making it suitable for various applications, including transportation and heating.

Syngas Production: In the production of synthesis gas (syngas) from coal, natural gas, or other feedstocks, the Rectisol process can be used to remove contaminants like CO_2 and H_2S to improve the quality of the syngas for subsequent chemical reactions.

Hydrogen Production: In hydrogen production processes, such as steam methane reforming (SMR) or gasification of hydrocarbons, rectisol can be used to purify the hydrogen stream by removing impurities like CO_2 and H_2S.

Carbon Capture and Storage (CCS): Rectisol can be applied in carbon capture processes to capture CO_2 emissions from power plants or industrial facilities before they are released into the atmosphere. The captured CO_2 can be transported and stored underground to reduce greenhouse gas emissions.

Ammonia Production: In the production of ammonia, rectisol can be used to purify the synthesis gas by removing CO_2 and H_2S, which can otherwise interfere with the ammonia synthesis reaction.

Refinery Gas Cleanup: The Rectisol process can be used to remove contaminants like H_2S and CO_2 from refinery off-gases, improving the quality of the gas streams and preventing environmental emissions.

Biogas Upgrading: Rectisol can be employed in the purification of biogas, which is produced from organic waste materials. This process helps remove impurities and produces cleaner biogas suitable for use as a renewable energy source.

Petrochemical Industry: Rectisol can be used for gas purification in various petrochemical processes, ensuring that impurities are removed from the feed gases to prevent equipment corrosion and maintain product quality.

Environmental Control: The Rectisol process can also be used for environmental control in industries where emissions of CO_2 and H_2S are regulated to reduce environmental impact.

Overall, the Rectisol wash process is a versatile technology for gas purification and is commonly used in industries where the removal of specific impurities from gas streams is necessary for process efficiency, environmental compliance, and product quality.

Assuming the feed consists of an impure gas mixture consisting of carbon dioxide and hydrogen sulfide as major impurities, Then the model submitted by Mr. Vanddanti Goutham, which can be accessed from [40], shows the results as shown in Table 45 for the model shown in Figure 51 below.

According to the abstract for the process model, this process flowsheet for the Rectisol process was developed using DWSIM (Ver 7.3.1), taking reference from Figure 4 of [39]. The crude syngas at about -20.59 ºC and 34 bar pressure and the pure methanol at -50 ºC and 44 bar pressure were supplied to an absorption column (Chemsep). The absorption column has 60 stages. The Peng Robinson property package is used for the entire process. The top product from the column is obtained at -47.57 ºC and consists of purified syngas with more than 99% H_2S removed. The CO_2-rich stream is drawn from the middle of the column and flashed at 11 bar and 5 bar, respectively, to remove CO_2. The bottom product from the Chemsep column is flashed at 12 bars to remove H_2 and CO. The CO_2-devoid middle stream and the H_2S-rich bottom product are stripped with N_2 at a reduced pressure of about 0.2 bar to remove the absorbed CO_2 as tail gas. The H2S-rich stream from this column is subjected to distillation to separate H_2S and meth.anol.

The absorber column was fed with methanol of mass flow rate 163990.24 kg/h at the inlet stream ‘S-02’ in order to absorb the impure compounds from the stream ‘S-01’.

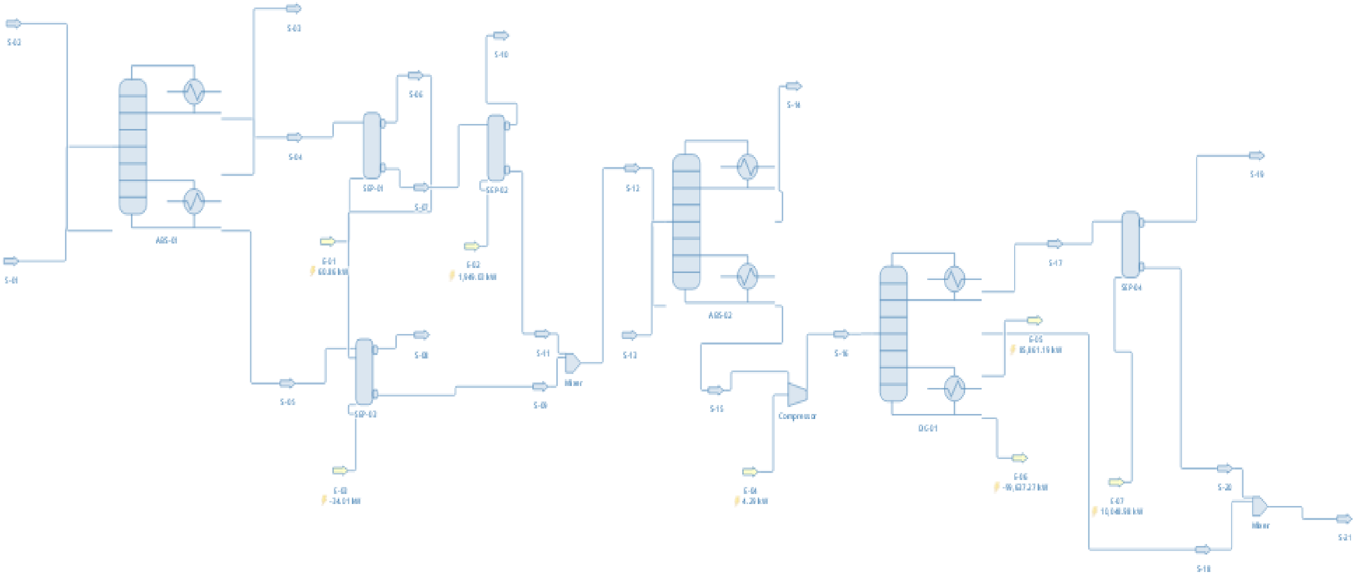


Figure 51: Simulation model for Rectisol wash process

The above simulation had the following components at the outlet streams: ‘S-03, S-10, S-14, S-19, S-21, and S-08’. These streams had the following mass flow rate of products for the mass flow rate of different components as the fed compounds at stream ‘S-01’.

Table 45: Mass flow rate at different streams

S-01 (feed)	**Mass flow rate (kg/h)**	S-03	Mass flow rate (kg/h) of vapor	S-10	Mass flow rate (kg/h) of vapor	S-14	Mass flow rate (kg/h) of vapor
Argon	**192.396**	Argon	186.5632	Argon	1.542163	Argon	639.5805
Hydrogen	**3920.11**	Hydrogen	3906.047	Hydrogen	0.620513	Hydrogen	32.61696
Nitrogen	**331.0848**	Nitrogen	324.3057	Nitrogen	1.36908	Nitrogen	449.1946
Carbon monoxide	**22474.46**	Carbon monoxide	22284.71	Carbon monoxide	18.73343	Carbon monoxide	457.1629
Methane	**121.8874**	Methane	116.5109	Methane	1.792569	Methane	256.7852
Carbon dioxide	**63510.89**	Carbon dioxide	1729.427	Carbon dioxide	25570.26	Carbon dioxide	34371.63
Hydrogen sulfide	**185.5735**	Hydrogen sulfide	1.07E-18	Hydrogen sulfide	0.196164	Hydrogen sulfide	159.4516
Methanol	**39.08687**	Methanol	2.518045	Methanol	34.77369	Methanol	296.9489

S-19	Mass flow rate (kg/h) of vapor	S-08	Mass flow rate (kg/h) of vapor	S-21	Mass flow rate (kg/h) of liquid
Argon	8.16E-05	Argon	3.644572	Argon	0.003565
Hydrogen	5.90E-06	Hydrogen	13.18881	Hydrogen	3.55E-06
Nitrogen	5.58E-05	Nitrogen	4.846517	Nitrogen	0.001263
Carbon monoxide	1.71E-05	Carbon monoxide	163.289	Carbon monoxide	0.000212
Methane	0.000125	Methane	2.820735	Methane	0.003199
Carbon dioxide	0.00517	Carbon dioxide	2361.98	Carbon dioxide	2.243535

Hydrogen sulfide	0.019737	Hydrogen sulfide	5.794646	Hydrogen sulfide	27.01575
Methanol	0.974807	Methanol	1.630915	Methanol	139114.6

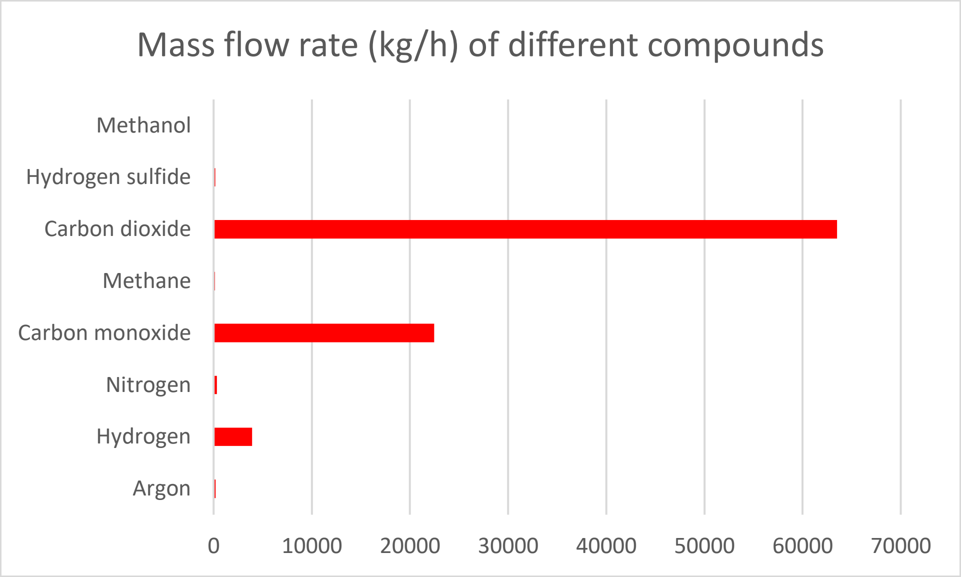


Figure 52: Mass flow rate of different compounds at the feed

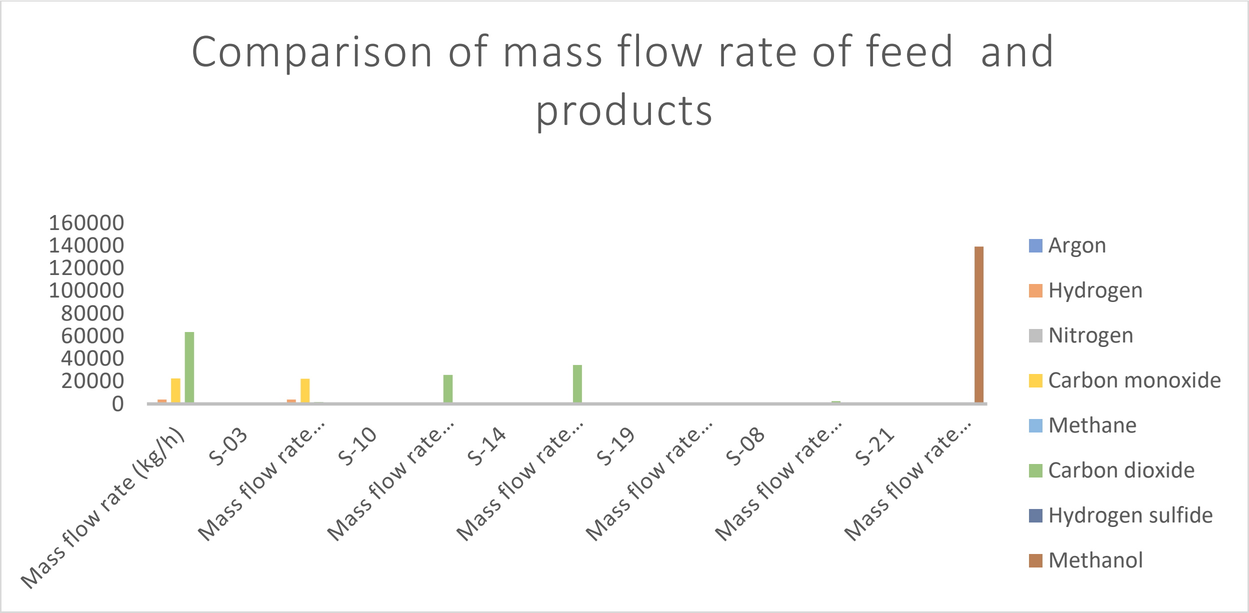


Figure 53: Comparison of mass flow of feed and products

Table 46: Mass and energy balance for different equipment used

Equipment	**Type**	**Energy Consumption (-) / Generation (+) (kW)**	**Efficiency (%)**	**MBR (kg/h)**	**EBR (kW)**
Mixer	Stream Mixer	0.00360321		2.55795E-11	-0.00360321
SEP-04	Gas-Liquid Separator	-10049		0.00128045	-0.00910145
Compressor	Compressor	-4.28747	100	0	9.48575E-13
ABS-02	CAPE-OPEN Unit Operation	-45.6546		-2.01025	45.6546
Mixer	Stream Mixer	-0.000384066		0	0.000384066
SEP-03	Gas-Liquid Separator	34.0075		0.0203909	0.130448
SEP-02	Gas-Liquid Separator	-1949.03		0.28336	1.26735
SEP-01	Gas-Liquid Separator	-60.8622		0.00905372	0.0507143
ABS-01	CAPE-OPEN Unit Operation	-0.0230767		1.53477E-10	0.0230767

The above results show that the process is complex and many impure gases get released with a large quantity of pure gas mixture. The collection of all of the impure gases may be more costly, and the modeled system cannot be said to be a highly effective process for separating impure H_2 and CO_2.

The same process can be designed, but with the addition of a cooler and compressor, cryogenic compression technology, and recyclers, in order to save time and energy and increase the efficiency of the overall process.

Setting the base location as India, the DWSIM capital cost estimator was used to determine the value of CAPEX and OPEX, including the cost of used methanol in the year 2023 for the absorption of impure H_2S and CO_2 for the above process model, which are mentioned in the below table:

Table 47: Cost estimation parameters

Cost index	Value
CAPEX	$3,675,906.98
OPEX	$1,440,973,682.26/year

The OPEX for the built model is very high and is not a feasible method to be implemented in the separation and purification of gases in process industries.

Rather, a more cost-efficient model than the above model in Figure 51 can be proposed, consisting of cryogenic compression and recycling technology. The model had been developed with a single compressor, cooler, and absorption unit but was found to be effective in the separation of the individual impure components. Methanol at a feed flow rate of 15000 kg/h was fed into the 'Methanol' stream. The flowsheet of the developed model is shown below:

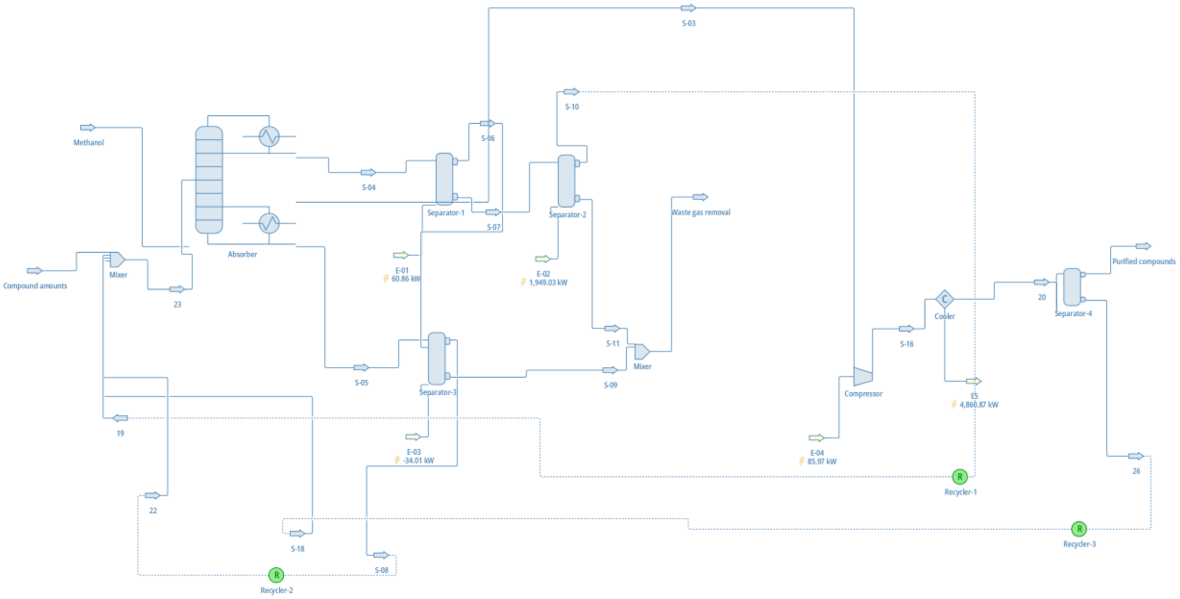


Figure 54: Modified simulation model of Rectisol process

The above model was built using the components at the 'Compound amounts' stream as mentioned in Table 46 below.

Table 48: Mass flow rate of compounds

Compounds	Mass flow rate (kg/h)
Argon	192.396
Hydrogen	3920.1099
Nitrogen	331.08477
Carbon monoxide	22474.461
Methane	121.8874
Carbon dioxide	63510.888
Hydrogen sulfide	185.57346
Methanol	39.086872

The Peng-Robinson property package was used for every component used in building the above process model. The 'compound amounts' stream consisted of a fed impure and pure gas mixture, as shown in Table 46 above. The mass and energy balance involved for every piece of equipment and stream used are as follows:

Table 49: Mass and energy balance for different equipment

Equipment	**Type**	**Energy Consumption (-) / Generation (+) (kW)**	**Efficiency (%)**	**MBR (kg/h)**	**EBR (kW)**
Absorber	CAPE-OPEN Unit Operation	-70652.3		37919.8	70652.3
Separator-1	Gas-Liquid Separator	-60.8622		0.00905372	0.0507143
Separator-2	Gas-Liquid Separator	-1949.03		0.28336	1.26735
Separator-3	Gas-Liquid Separator	34.0075		0.0203909	0.130448
Mixer	Stream Mixer	-0.000384066		0	0.000384066
Separator-4	Gas-Liquid Separator	-1.58832		1.25285	1.58832
Mixer	Stream Mixer	0.0157547		0	-0.0157547
Compressor	Compressor	-85.9704	100	0	8.3844E-13
Cooler	Cooler	4860.58	100	0	0.284538

Table 50: Mass and energy balance at streams

Name	Mass Flow (kg/h)	Temperature (°C)	Pressure (bar)	Energy Flow (kW)
26	23723.6	-203.58	35	-30957.1
Purified compounds	4825.25	-203.58	35	-4402.29
20	28550.1	-203.58	35	-35361
S-18	23723.6	-203.58	35	-30957.1
Methanol	150000	-50	44	-324692
Compound amounts	90775.5	-20.59	34	-184885
S-03	28550.1	-47.5745	33	-30586.4
S-04	175681	-17.9697	33	-395549
S-05	50534.7	-19.207	33	-113726
S-06	2543.05	-17.9697	11	-6127.39
S-07	173138	-17.9697	11	-389360
S-10	25629.3	-17.9697	5	-63887.9
S-11	147508	-17.9697	5	-323522
S-08	2557.2	-19.1477	12	-6090.79
S-09	50520.6	-19.1477	12	-113796
Waste gas removal	198029	-18.3574	8.5	-437318
22	2557.2	-19.1477	12	-6090.8
23	142686	-78.6631	5	-285821
S-16	28550.1	-43.5797	35	-30500.4
19	25629.3	-17.9697	5	-63887.9

The stream 'Waste gas removal' produced the following components, all of which were liquids: carbon dioxide, hydrogen sulphide, and methanol, which were separated from the fed gas mixture.

Table 51: Generated of waste gases

Argon	0.64561445
Hydrogen	0.25196674
Nitrogen	0.56287739
Carbon monoxide	7.7128191
Methane	0.76285855
Carbon dioxide	33847.978
Hydrogen sulfide	179.58285
Methanol	163991.35

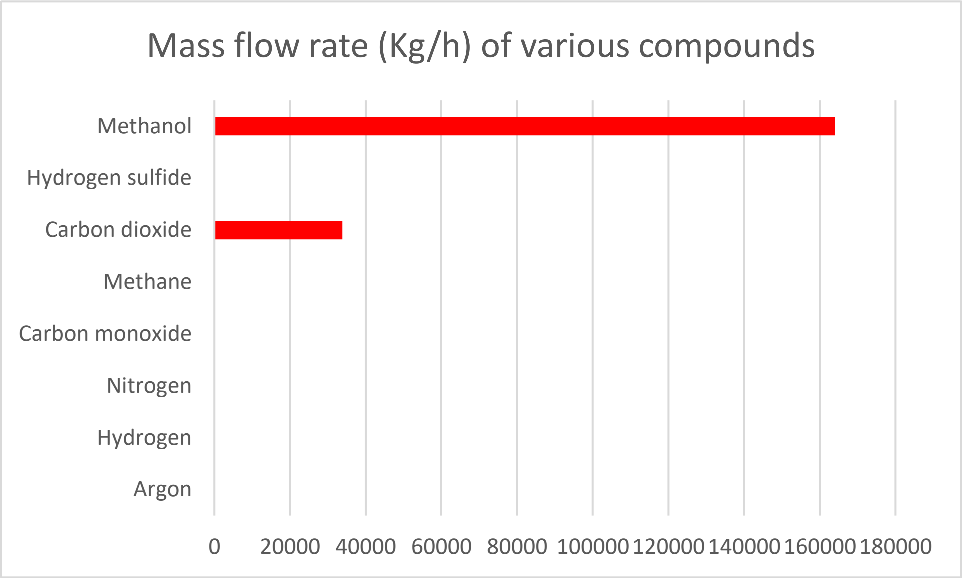
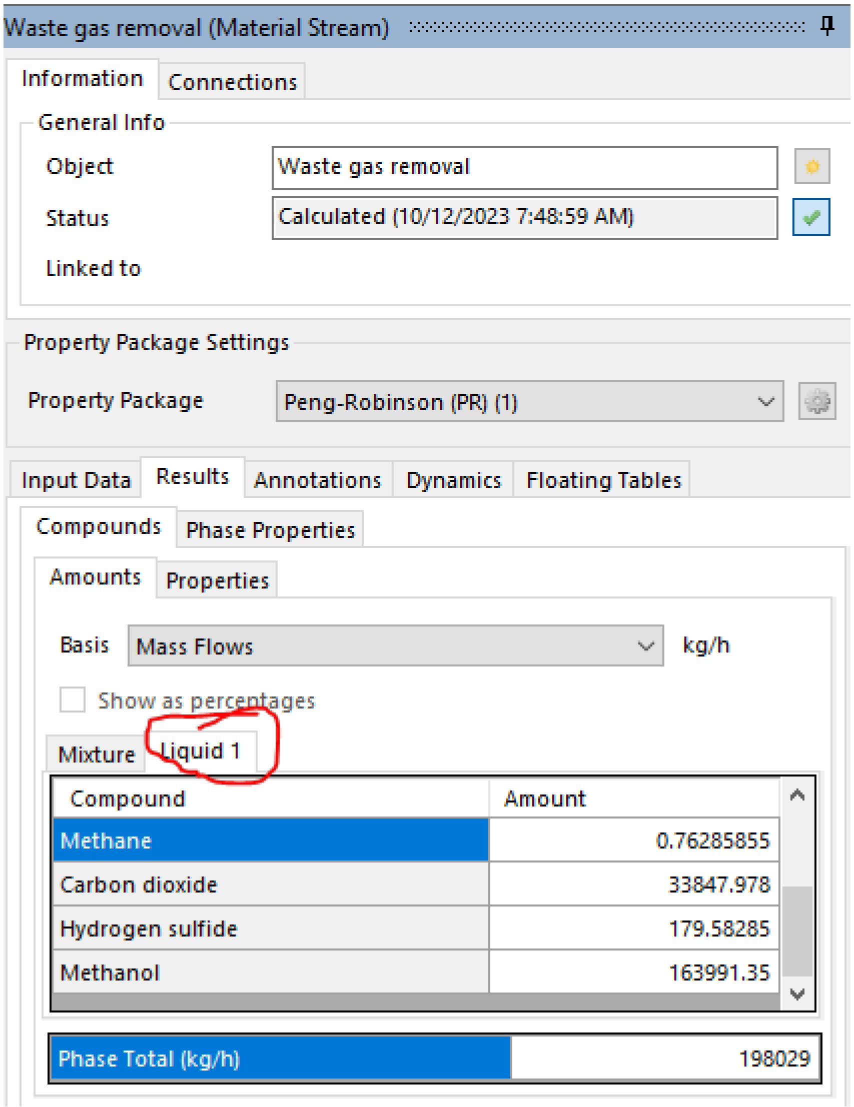


Figure 55: Mass flow rate of various compounds at 'Purified compounds' stream

Similarly, the mass flow rates of different components in the 'waste gas removal' stream and 'purified compounds' were compared, due to which the following results were obtained:

Table 52: Comparison of impure and pure compounds' mass flow

Waste gas removal stream Compounds	Impure compound's Mass flow rate (kg/h)	Pure compound's Mass flow rate (kg/h)
Argon	0.6456145	4.374268
Hydrogen	0.2519667	3846.192
Nitrogen	0.5628774	32.67791
Carbon monoxide	7.7128191	941.6574
Methane	0.7628586	0.343664
Carbon dioxide	33847.978	0.000469
Hydrogen sulfide	179.58285	2.99E-25
Methanol	163991.35	1.15E-17



Waste gas removal (Material Stream)

Object: Waste gas removal

Status: Calculated (10/12/2023 7:48:59 AM)

Linked to

Property Package Settings

Property Package: Peng-Robinson (PR) (1)

Basis: Mass Flows kg/h

☐ Show as percentages

Compound	Amount
Methane	0.76285855
Carbon dioxide	33847.978
Hydrogen sulfide	179.58285
Methanol	163991.35

Phase Total (kg/h): 198029

Figure 56: Liquid product at outlet

Similarly, to obtain the pure components as shown in Figure 56 above, the cooler and compressor were used with specifications as shown in Table 48 above. The stream 'Purified Components' has been used as an outlet stream to recover the purified compounds with very small amounts of impure components present in the vapor form.

Table 53: Mass flow rate of purified and impure compounds

Compounds	Mass flow rate (kg/h)
Argon	4.374268

Hydrogen	3846.192
Nitrogen	32.67791
Carbon monoxide	941.6574
Methane	0.343664
Carbon dioxide	0.000469
Hydrogen sulfide	2.99E-25
Methanol	1.15E-17

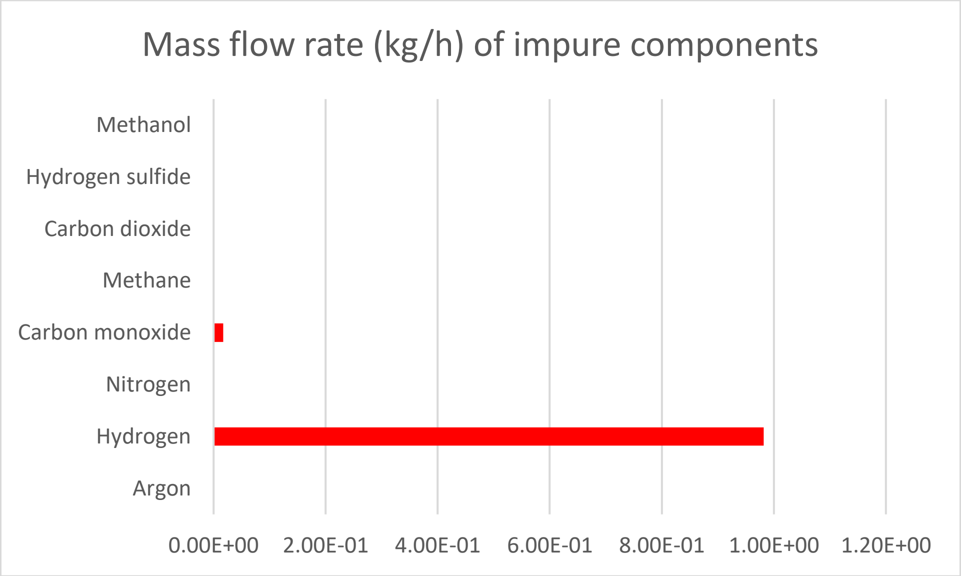
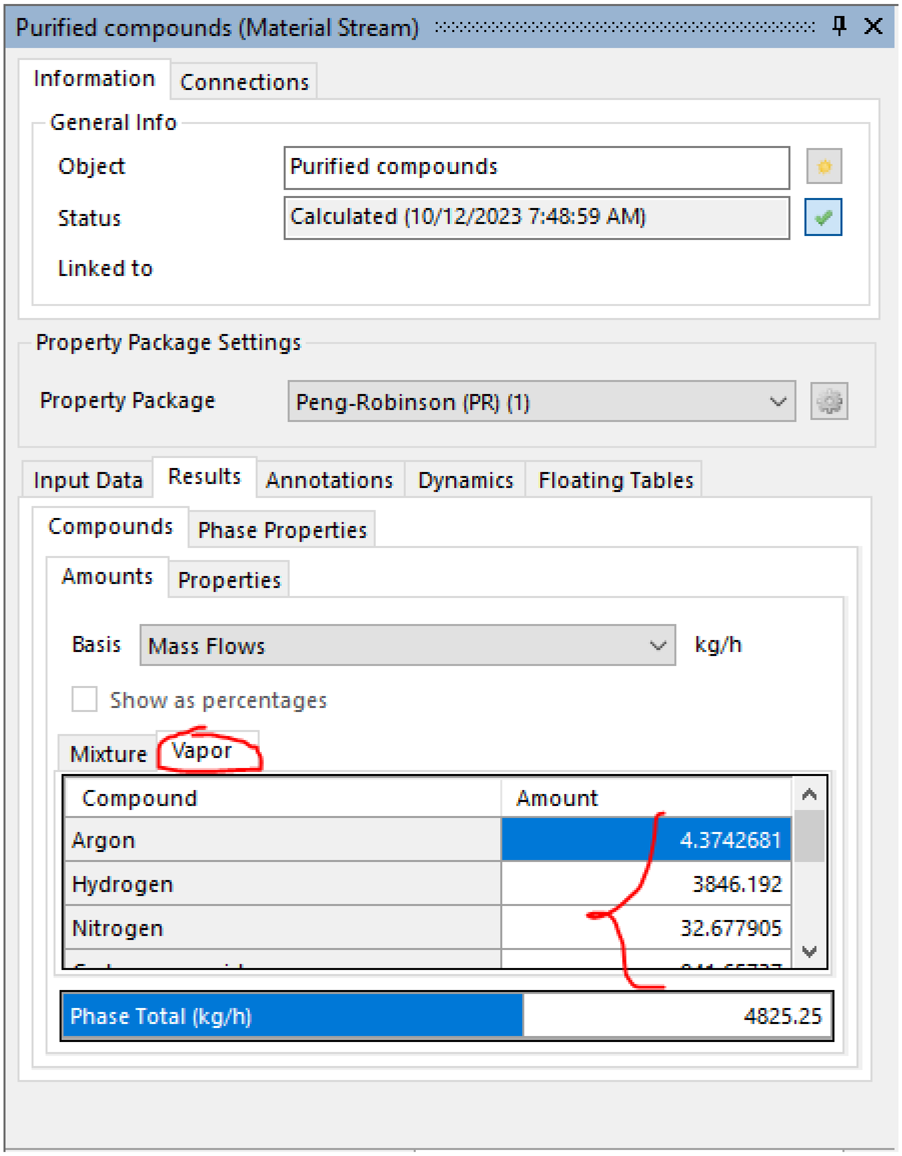


Figure 57: Mass flow rate of impure components



General Info

Object: Purified compounds

Status: Calculated (10/12/2023 7:48:59 AM)

Linked to

Property Package Settings

Property Package: Peng-Robinson (PR) (1)

Basis: Mass Flows kg/h

☐ Show as percentages

Compound	Amount
Argon	4.3742681
Hydrogen	3846.192
Nitrogen	32.677905

Phase Total (kg/h)	4825.25

Figure 58: Mass flow rate of purified compounds

6.2. Comparison of two streams' components

The stream 'Waste gas removal' where the waste gases in liquid form are retained can be compared with the stream 'Purified compounds' where the pure gases are obtained. The following Table 52 and Figure 59 show the results obtained.

Table 54: Mass flow rate of pure and impure compounds

Waste gas removal stream Compounds	Impure compound's Mass flow rate (kg/h)	Pure compound's Mass flow rate (kg/h)
Argon	0.6456145	4.374268
Hydrogen	0.2519667	3846.192
Nitrogen	0.5628774	32.67791
Carbon monoxide	7.7128191	941.6574
Methane	0.7628586	0.343664
Carbon dioxide	33847.978	0.000469
Hydrogen sulfide	179.58285	2.99E-25
Methanol	163991.35	1.15E-17

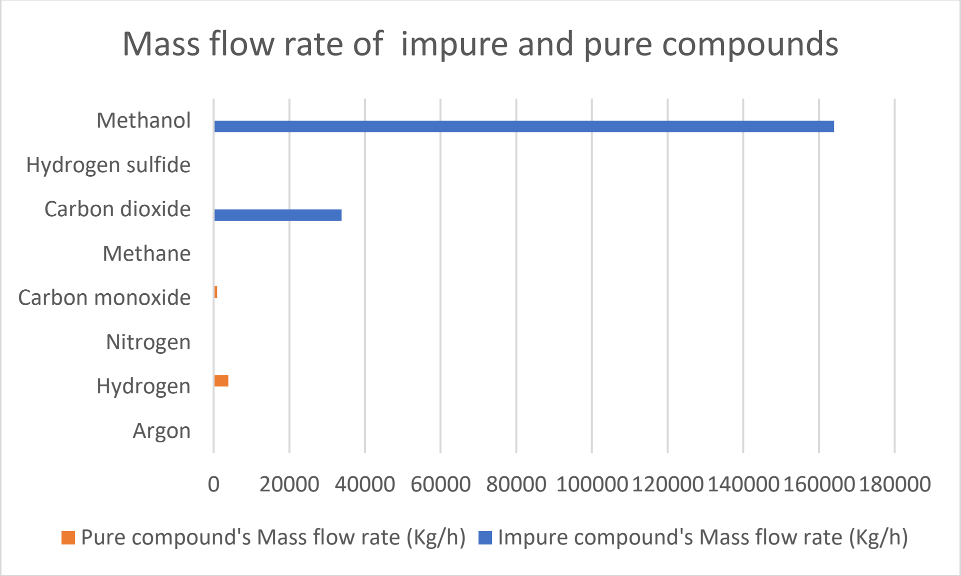


Figure 59: Mass flow rate of impure and pure compounds

6.3. Sensitivity analysis for the model proposed in Figure 54

The mass flow of several compounds at the ‘Compound amounts’ stream is varied with the mass flow of methanol at the ‘Methanol’ stream and the mass flow rate at the ‘Water gas removal’ stream for the compounds recovered at the liquid phase, due to which the following data and the graph plot were obtained.

Table 55: Sensitivity analysis for proposed model

Compound amounts - Mass Flow (kg/h)	Methanol - Mass Flow (kg/h)	Waste gas removal - Mass Flow (Overall Liquid) (kg/h)
80000	130000	198029
80000	137500	198029
80000	145000	198029
80000	152500	198029
80000	160000	198029
83000	130000	198029
83000	137500	198029
83000	145000	198029
83000	152500	198029
83000	160000	198029
86000	130000	198029
86000	137500	198029
86000	145000	198029
86000	152500	198029
86000	160000	198029
89000	130000	198029
89000	137500	198029
89000	145000	198029
89000	152500	198029
89000	160000	198029
92000	130000	198029
92000	137500	198029
92000	145000	198029
92000	152500	198029
92000	160000	198029

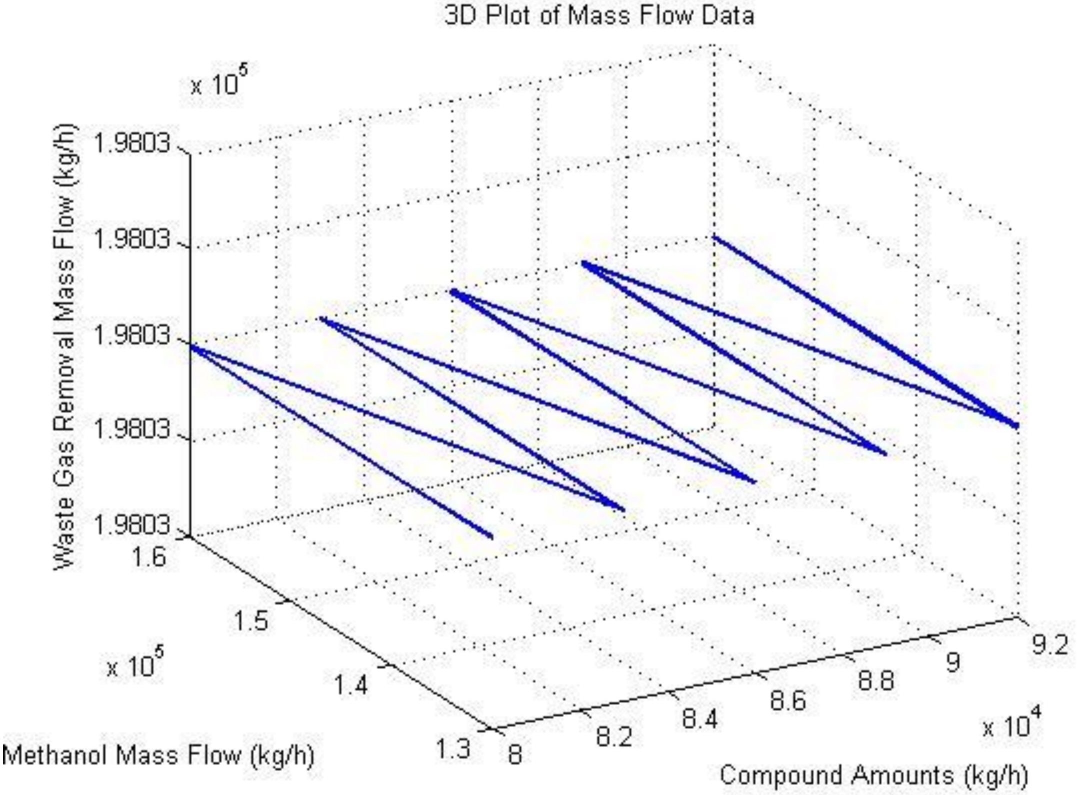


Figure 60: 3D plot for mass flow rate of water gas removal vs methanol mass flow vs compound amount

Thus, the above results show that the small variation in the methanol and impure gas mixture in fed has no effect on the obtained liquid composition of waste gases in the 'Waste Gas Removal' stream.

Similarly, the mass flow rate of pure components recovered at the 'Purified Compounds' stream is varied by the variation of mass flow of several compounds at the 'Compound Amounts' stream, which is varied with the mass flow of methanol at the 'Methanol' stream, through which the following results were obtained.

Table 56: Sensitivity analysis for proposed model

Compound amounts - Mass Flow (kg/h)	Methanol - Mass Flow (kg/h)	Purified compounds - Mass Flow (Vapor) (kg/h)
80000	130000	4825.25

80000	137500	4825.25
80000	145000	4825.25
80000	152500	4825.25
80000	160000	4825.25
83000	130000	4825.25
83000	137500	4825.25
83000	145000	4825.25
83000	152500	4825.25
83000	160000	4825.25
86000	130000	4825.25
86000	137500	4825.25
86000	145000	4825.25
86000	152500	4825.25
86000	160000	4825.25
89000	130000	4825.25
89000	137500	4825.25
89000	145000	4825.25
89000	152500	4825.25
89000	160000	4825.25
92000	130000	4825.25
92000	137500	4825.25
92000	145000	4825.25
92000	152500	4825.25
92000	160000	4825.25

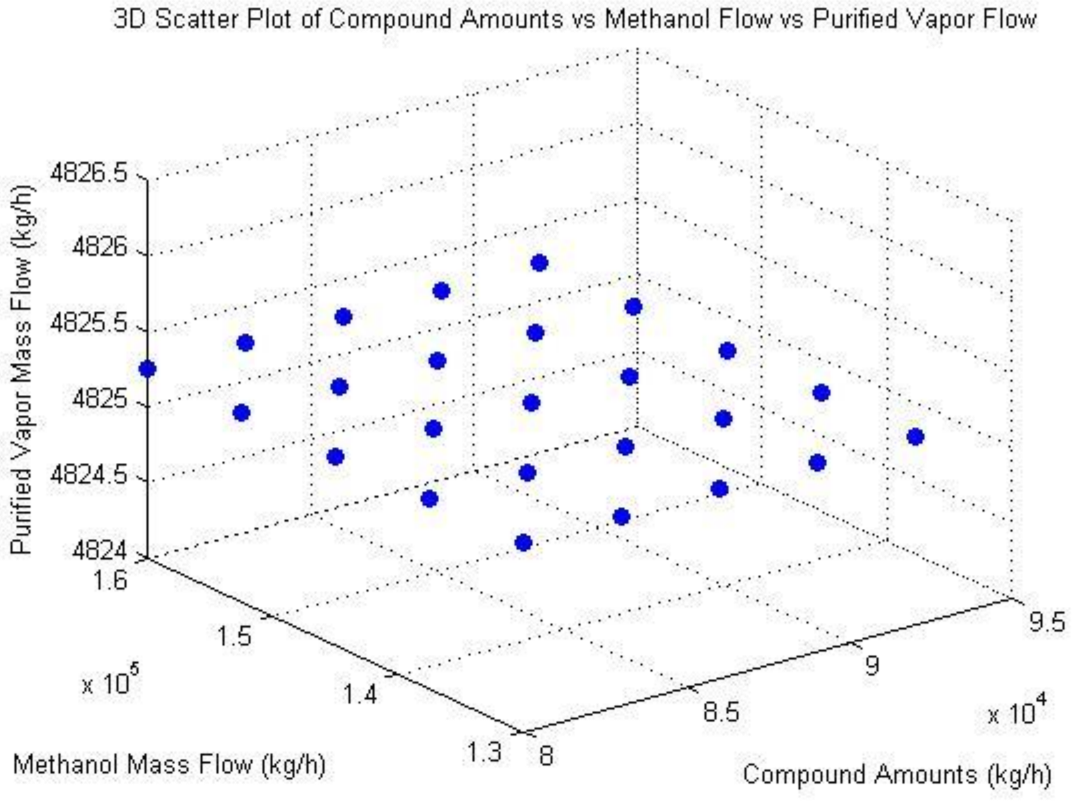


Figure 61: Plot for compound amounts vs methanol mass flow vs purified vapor's mass flow

The cost estimation was done for both the model from [31] and the modified model in Figure 54 using the DWSIM's capital cost estimator, setting the base location as India, due to which the following results were obtained: the OPEX was calculated by adding the methanol's cost that had been fed for retrieving the pure compounds separated from impure compounds.

Table 57: Parameters for expenses

Model	CAPEX	OPEX
Figure 51 from [31]	\$3,675,868.42	\$1,440,973,669.50/year
Figure 54 (Modified model)	\$5,130,147.19	\$1,318,900,086.61/year

Despite the cost of the model proposed by us is higher than that accessed in [40], but the proposed model is highly efficient in recovering the impure and pure components at different streams than the model accessed from [40].

6.4. Application in Methanol Formation

Methane is a highly useful hydrocarbon gas with several important uses in various industries and applications. Here are some of the key uses of methane:

1) **Natural Gas:** Methane is the major component of natural gas, which is used for heating, cooking, and generating electricity in homes and industries and has high calorific value.
2) **Fuel:** Methane can be used as a clean-burning fuel in compressed natural gas (CNG) and liquefied natural gas (LNG) vehicles. It is considered an eco-friendly alternative to gasoline and diesel as it produces fewer emissions when burned.
3) **Chemical Feedstock:** Methane can be as a raw material for the production of various chemicals and compounds, that include hydrogen, ammonia, methanol, and synthetic natural gas.
4) **Power Generation:** Methane can be used in power plants to generate electricity through gas turbines or combined-cycle power plants. It is a highly effective and low-emission fuel for electricity generation.
5) **Heating and Cooling:** Methane can be used in cogeneration or combined heat and power (CHP) systems to simultaneously produce electricity and heat, making it an efficient source for heating and cooling buildings.
6) **Agriculture:** In agriculture, methane is produced by the anaerobic decomposition of organic matter, such as livestock manure and food waste. It can be harnessed to generate renewable energy through technologies like biogas digesters.
7) **Wastewater Treatment:** Wastewater treatment plants can capture and use methane produced during the treatment process to generate electricity, heat, or steam, reducing operating costs.
8) **Rocket Propulsion:** Methane has been considered as a potential rocket fuel due to its high energy density and the possibility of producing it on other celestial bodies, such as Mars, for future space missions. Recently, agencies like SpaceX and Nasa have used the fuel in their rocket propulsion.
9) **Industrial Processes:** Methane can be used as a reducing agent in certain industrial processes, such as metal production and chemical manufacturing.
10) **Refrigeration:** Methane can be used as a refrigerant in some industrial cooling and refrigeration systems.
11) **Leak Detection:** Methane detectors are used to identify leaks in natural gas pipelines, as methane is a major component of natural gas.
12) **Research and Laboratory Applications:** Methane is used in various scientific and laboratory experiments, such as in mass spectrometry and isotope analysis.

The liquid form of carbon dioxide obtained from carbon capture processes can also be used for methanol synthesis by mixing with various other gases.

The in-built model of methanol synthesis by CO_2 hydrogenation in DWSIM developed by the DWSIM development team can be an example. This overall methanol generation plant provided in DWSIM’s sample can be taken as an example to explain the use of CO_2 captured. The captured CO_2 in liquid form can be converted to gasified form by high pressure and heating. Thus, as explained in the in-built model, the CO_2 can be used for the generation of commercial methanol. At the inlet streams at different points of the overall process model, the following composition (mass flow rate in kg/h) for individual components was used:

Table 58: Composition of inlet streams

CO_2	Mass flow rate (kg/h)	CW_1	Mass flow rate (kg/h)	CW_2	Mass flow rate (kg/h)
Methanol	0.0001	Methanol	0	Methanol	0
Water	0.0001	Water	3600	Water	3600
Hydrogen	0.05	Hydrogen	0	Hydrogen	0
Carbon dioxide	0.7996	Carbon dioxide	0	Carbon dioxide	0
Carbon monoxide	0.04	Carbon monoxide	0	Carbon monoxide	0
Nitrogen	0.0001	Nitrogen	0	Nitrogen	0
Oxygen	0.0001	Oxygen	0	Oxygen	0
Argon	0.11	Argon	0	Argon	0
CW3	Mass flow rate (kg/h)	Hydrogen	Mass flow rate (kg/h)	CW4	Mass flow rate (kg/h)
Methanol	0	Methanol	0.126367	Methanol	0
Water	3600	Water	39.0761	Water	10000
Hydrogen	0	Hydrogen	105.4604	Hydrogen	0
Carbon dioxide	0	Carbon dioxide	83.95391	Carbon dioxide	0
Carbon monoxide	0	Carbon monoxide	53.81638	Carbon monoxide	0
Nitrogen	0	Nitrogen	0.110481	Nitrogen	0
Oxygen	0	Oxygen	0.126197	Oxygen	0
Argon	0	Argon	17.33014	Argon	0

The process model with the mas and energy balance at the various streams and equipment for the model are mentioned below:

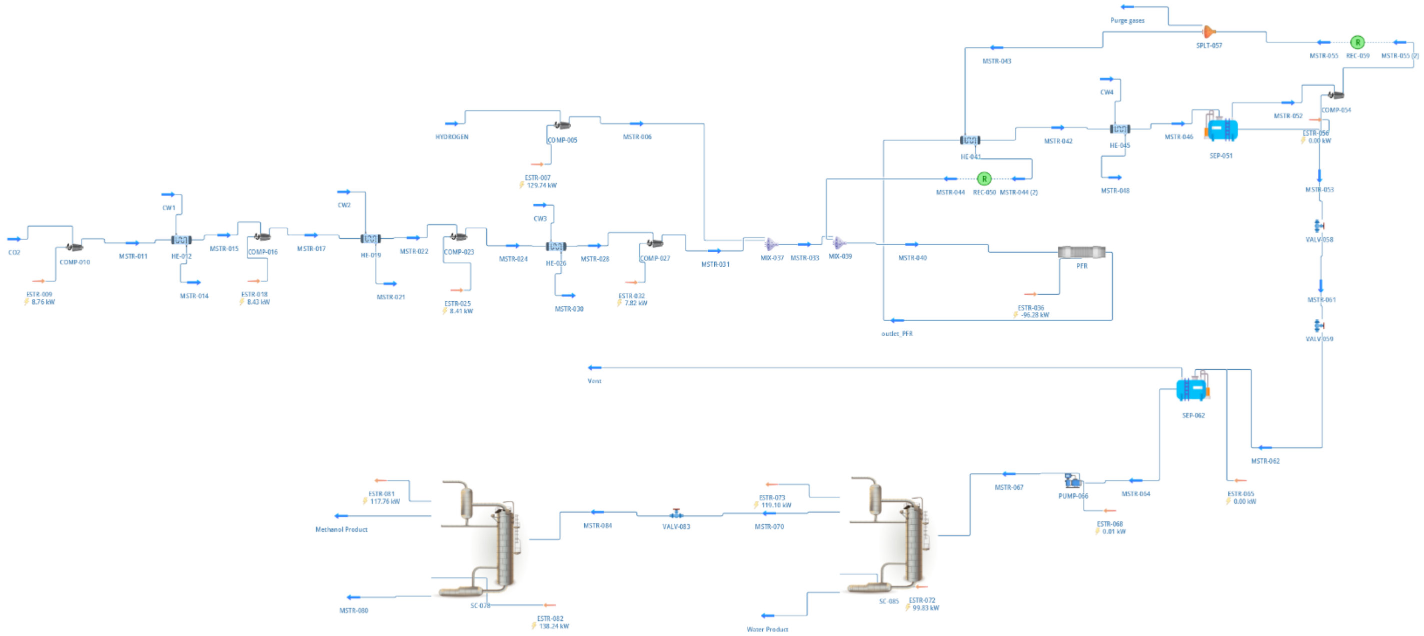


Figure 62: Inbuilt model of Methanol synthesis by CO_2 Hydrogenation in DWSIM

Table 59: Mass and energy balance of various equipment

Equipment	**Type**	**Energy Consumption (-) / Generation (+) (kW)**	**Efficiency (%)**	**MBR (kg/h)**	**EBR (kW)**
SC-085	Shortcut Column	19.2702		0.00843572	0.0147975
COMP-005	Compressor	-129.74	75	0	-1.06749E-08
PFR	Plug-Flow Reactor (PFR)	96.2826		0.000142175	4.53326E-12
COMP-010	Compressor	-8.75675	75	0	2.25532E-06
HE-012	Heat Exchanger	1.13687E-09	100.004	0	-1.13687E-09
COMP-016	Compressor	-8.43238	75	0	2.31438E-07

Equipment	Type	Energy Consumption (-) / Generation (+) (kW)	Efficiency (%)	MBR (kg/h)	EBR (kW)
HE-019	Heat Exchanger	2.02272E-09	100.002	0	-2.02272E-09
COMP-023	Compressor	-8.4138	75	0	2.14731E-07
HE-026	Heat Exchanger	-3.39351E-08	99.9994	0	3.39351E-08
COMP-027	Compressor	-7.82066	75	0	-6.41497E-07
MIX-037	Stream Mixer	-2.515E-08		6.99441E-13	2.515E-08
MIX-039	Stream Mixer	0.00446118		-0.0199051	-0.00446118
HE-041	Heat Exchanger	-9.89075E-12	78.6065	-4.996E-14	9.89075E-12
HE-045	Heat Exchanger	-0.00088189	65.5568	0	0.00088189
SEP-051	Gas-Liquid Separator	-0.0431457		0.0142148	0.0431457
COMP-054	Compressor	0.00122139	75	0	-8.11628E-06
SPLT-057	Stream Splitter	14.1146		-6.89915	-14.1146
VALV-058	Valve	-3.5471E-07		0	3.5471E-07
VALV-059	Valve	3.25001E-05		0	-3.25001E-05
SEP-062	Gas-Liquid Separator	0		-6.94788E-05	-2.33904E-05
PUMP-066	Pump	-0.0105427	75	0	2.17456E-08
VALV-083	Valve	1.03756E-09		0	-1.03756E-09
SC-078	Shortcut Column	-20.4764		0.00228897	0.00399209

For streams:

Table 60: Mass and energy balance at different streams

Name	Mass Flow (kg/h)	Temperature (°C)	Pressure (bar)	Energy Flow (kW)
Water Product	105.724	96.3883	1.01325	0
MSTR-070	142.789	-88.458	1.01325	0
outlet_PFR	1028.71	237	73	0
MSTR-006	300	239.728	78	0

Name	Mass Flow (kg/h)	Temperature (°C)	Pressure (bar)	Energy Flow (kW)
HYDROGEN	300	25	10.75	0
CO2	300	41.6	1.01325	0
MSTR-011	300	158.148	3	0
CW1	3600	35	1.01325	0
MSTR-014	3600	37.0761	1.01325	0
MSTR-015	300	34.9945	3	0
MSTR-017	300	149.162	8.8	0
CW2	3600	35	1.01325	0
MSTR-021	3600	36.9533	1.01325	0
MSTR-022	300	34.9981	8.8	0
MSTR-024	300	152.073	26.3	0
MSTR-028	300	35.0007	26.3	0
CW3	3600	35	1.01325	0
MSTR-030	3600	37.1286	1.01325	0
MSTR-031	300	152.413	78	0
MSTR-033	600	224.918	78	0
MSTR-040	1028.71	215.858	73	0
MSTR-042	1028.71	181.118	73	0
MSTR-043	428.69	87.1504	73	0
MSTR-044	428.69	205.146	73	0
MSTR-046	1028.71	87.0876	73	0
CW4	10000	20	1.01325	0
MSTR-048	10000	36.4382	1.01325	0
MSTR-044 (2)	428.69	205.146	73	0
MSTR-052	758.618	87.0876	73	0
MSTR-053	270.077	87.0876	73	0
MSTR-055	758.618	87.0874	73	0
MSTR-055 (2)	758.618	87.0874	73	0
Purge gases	336.828	87.1504	73	0
MSTR-061	270.077	88.2685	10	0
MSTR-062	270.077	68.92	1.01325	0
Vent	21.5558	68.92	1.01325	0
MSTR-064	248.521	68.92	1.01325	0
MSTR-067	248.521	68.9359	2	0
MSTR-084	142.789	-88.458	1.01325	0
Methanol Product	141.916	59.6623	1.01325	0
MSTR-080	0.870524	87.2068	1.01325	0

The following results are obtained in the different outlet streams:

Table 61: Results at outlet streams

MSTR-014 (liquid)	Mass flow rate (kg/h)	MSTR-021 (liquid)	Mass flow rate (kg/h)	MSTR-030 (liquid)	Mass flow rate (kg/h)
Methanol	0	Methanol	0	Methanol	0
Water	3600	Water	3600	Water	3600
Hydrogen	0	Hydrogen	0	Hydrogen	0
Carbon dioxide	0	Carbon dioxide	0	Carbon dioxide	0
Carbon monoxide	0	Carbon monoxide	0	Carbon monoxide	0
Nitrogen	0	Nitrogen	0	Nitrogen	0
Oxygen	0	Oxygen	0	Oxygen	0
Argon	0	Argon	0	Argon	0
MSTR-048 (liquid)	Mass flow rate (kg/h)	Purge gases (vapor)	Mass flow rate (kg/h)	Purge gases (liquid)	Mass flow rate (kg/h)
Methanol	0	Methanol	32.12649	Methanol	0.000658
Water	10000	Water	5.814405	Water	0.000446
Hydrogen	0	Hydrogen	74.90296	Hydrogen	2.61E-07
Carbon dioxide	0	Carbon dioxide	162.059	Carbon dioxide	2.31E-05
Carbon monoxide	0	Carbon monoxide	12.14409	Carbon monoxide	3.98E-08
Nitrogen	0	Nitrogen	0.130939	Nitrogen	5.90E-10

Oxygen	0	Oxygen	0.149329	Oxygen	1.70E-09
Argon	0	Argon	49.49919	Argon	5.66E-07
Vent (Vapor)	Mass flow rate (kg/h)	Methanol Product (liquid)	Mass flow rate (kg/h)	Methanol Product (Vapor)	Mass flow rate (kg/h)
Methanol	13.62969	Methanol	8.66E-07	Methanol	141.6552
Water	2.430656	Water	1.75E-10	Water	0.079799
Hydrogen	0.062072	Hydrogen	1.29E-09	Hydrogen	2.73E-05
Carbon dioxide	5.288483	Carbon dioxide	2.36E-07	Carbon dioxide	0.183024
Carbon monoxide	0.009346	Carbon monoxide	1.25E-10	Carbon monoxide	4.01E-06
Nitrogen	0.00014	Nitrogen	1.44E-12	Nitrogen	8.57E-08
Oxygen	0.000406	Oxygen	9.00E-12	Oxygen	7.29E-07
Argon	0.134972	Argon	2.98E-09	Argon	0.000241
MSTR-080 (vapor)	Mass flow rate (kg/h)	MSTR-080 (liquid)	Mass flow rate (kg/h)		
Methanol	9.89E-05	Methanol	0.144744		
Water	6.48E-05	Water	0.729363		
Hydrogen	4.18E-58	Hydrogen	1.73E-59		
Carbon dioxide	3.57E-34	Carbon dioxide	1.81E-33		
Carbon monoxide	3.88E-55	Carbon monoxide	8.75E-57		
Nitrogen	4.02E-53	Nitrogen	9.74E-55		
Oxygen	4.06E-51	Oxygen	6.43E-52		
Argon	6.36E-49	Argon	1.00E-49		

6.5. Application in the electricity generation

The carbon dioxide generated can be converted to gaseous form from cryogenic compression and can be converted to useful electricity by the rotation of the turbine. The simulation model for the overall process of generating electricity from CO_2's upcycling plant is shown in the figure below:

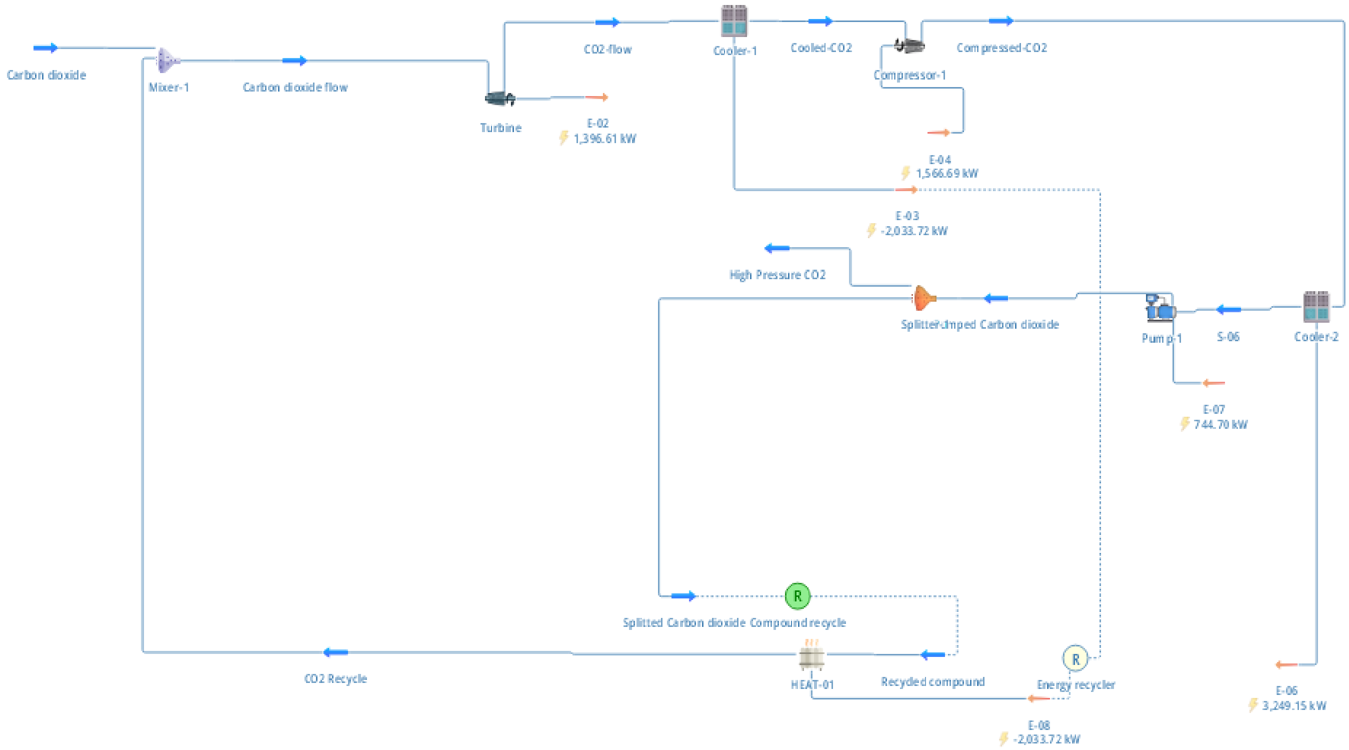


Figure 63: Electricity generation process simulation model using CO_2

The captured CO_2 in the proposed model in Figure 24 can be utilized to generate this useful electricity. Assuming the captured 14.89 kg/sec of liquid CO_2 is converted to the gaseous (vapor) form and then fed into the stream 'Carbon dioxide' as shown in the proposed model above in Figure 63, then, as shown in the figure, the turbine generates 1396.61 kW of electricity. The overall mass and energy balance for the whole equipment and the streams of this process model developed through DWSIM are as follows:

Table 62: Mass and energy balance for equipment used

Name	Mass Flow (kg/s)	Temperature (°C)	Pressure (bar)	Energy Flow (kW)
Recycled compound	0.474761	30.5384	300	-4240
CO_2 Recycle	0.474445	750	300	-3869.04
Splitted Carbon dioxide	0.474761	30.5384	300	-4242.83
High Pressure CO_2	14.8897	30.5384	300	-133065
Pumped Carbon dioxide	15.3644	30.5384	300	-137308

Name	Mass Flow (kg/s)	Temperature (°C)	Pressure (bar)	Energy Flow (kW)
S-06	15.3644	30	80	-138053
Compressed-CO_2	15.3644	206.599	80	-134804
Cooled-CO_2	15.3644	100	30	-136371
CO_2-flow	15.3644	-5.6325	30	-138404
Carbon dioxide flow	15.3644	53.4308	300	-137008
Carbon dioxide	14.89	25	1.01325	-133139

Table 63: Mass and energy balance for streams used

Name	Mass Flow (kg/s)	Temperature (°C)	Pressure (bar)	Energy Flow (kW)
Recycled compound	0.474761	30.5384	300	-4240
CO_2 Recycle	0.474445	750	300	-3869.04
Splitted Carbon dioxide	0.474761	30.5384	300	-4242.83
High Pressure CO_2	14.8897	30.5384	300	-133065
Pumped Carbon dioxide	15.3644	30.5384	300	-137308
S-06	15.3644	30	80	-138053
Compressed-CO_2	15.3644	206.599	80	-134804
Cooled-CO_2	15.3644	100	30	-136371
CO_2-flow	15.3644	-5.6325	30	-138404
Carbon dioxide flow	15.3644	53.4308	300	-137008
Carbon dioxide	14.89	25	1.01325	-133139

Similarly, the sensitivity analysis was performed to check the variation in values of dependent variables with the small change in the dependent variables.

Firstly, the mass flow rate of CO_2 was varied using ‘Carbon dioxide’ stream as inlet due to which following results were obtained for generated power at the turbine keeping all the other parameters except those present in the Table 61 constant.

Table 64: Result of sensitivity analysis

Carbon dioxide - Mass Flow (kg/s)	Turbine - Power Generated (kW)
0	0.127031
2.22222	208.43
4.44444	416.873
6.66667	625.316

Carbon dioxide - Mass Flow (kg/s)	Turbine - Power Generated (kW)
8.88889	833.759
11.1111	1042.2
13.3333	1250.65
15.5556	1459.09
17.7778	1667.53
20	1875.98

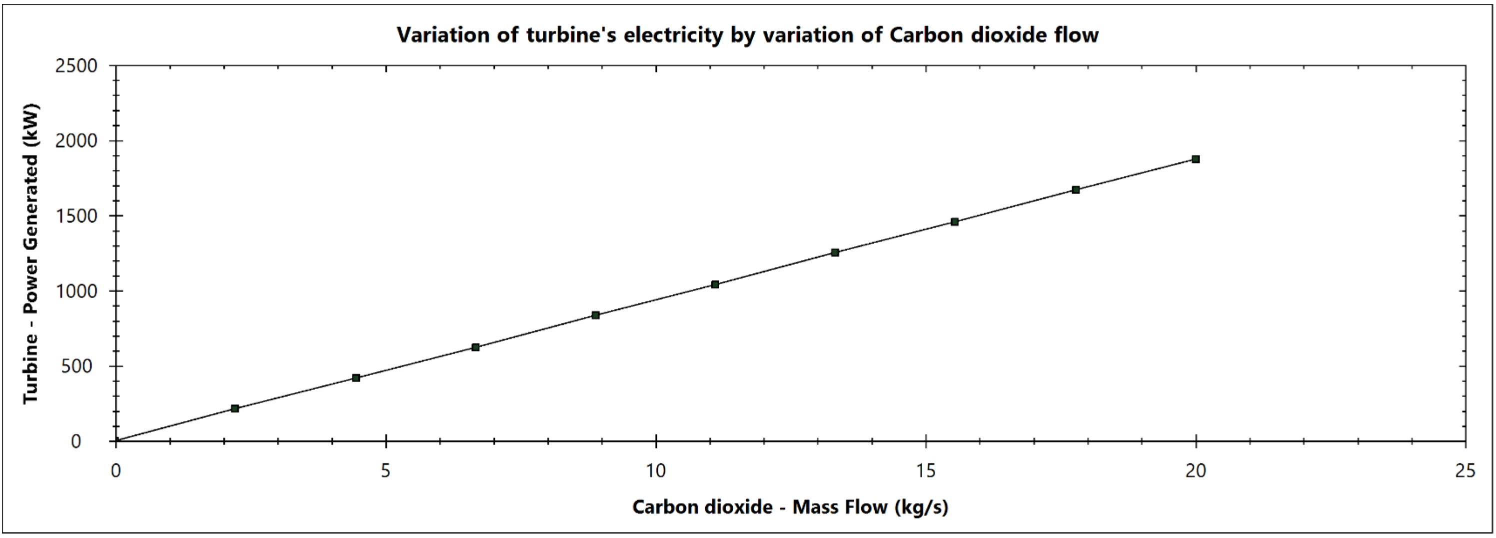


Figure 64: Carbon dioxide's mass flow rate vs power generation by turbine

Above results show that the turbine gives high electricity output with high variation in mass flow rate of carbon dioxide at feed stream 'Carbon dioxide'.

Similarly, the mass flow rate of CO_2 was varied for 'Carbon dioxide' stream and Cooler's outlet temperature as independent variables due to which following results were obtained for generated power at the turbine as dependent variable keeping all the other parameters constant as presented in the Table 68.

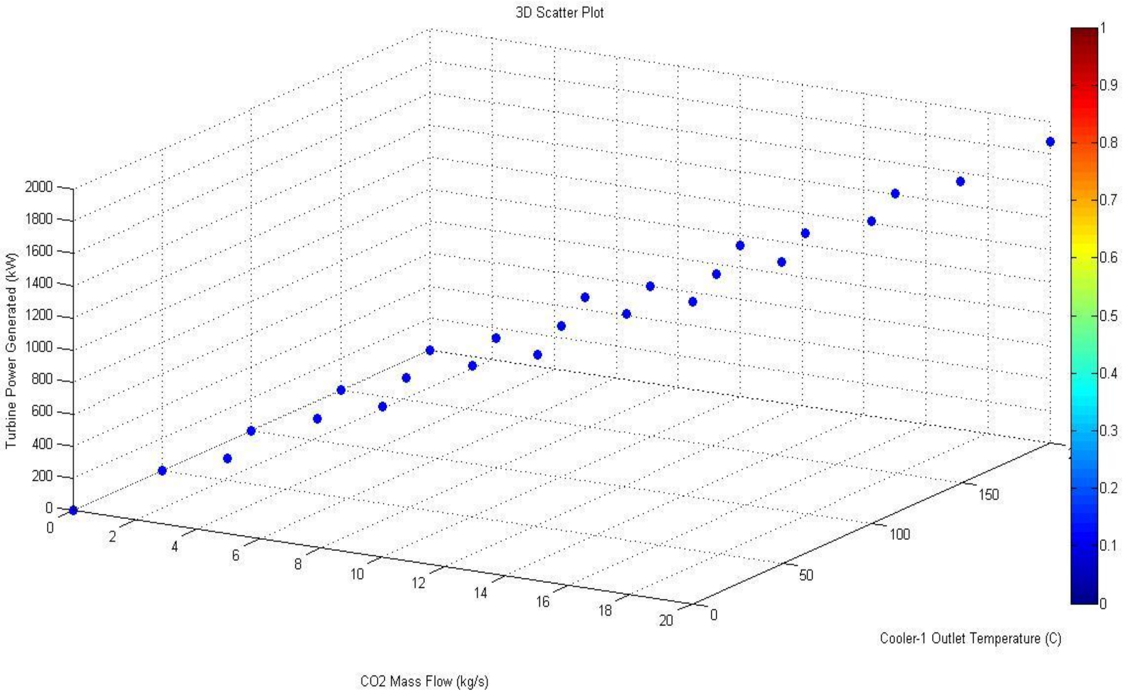


Figure 65: CO_2's mass flow rate and Cooler-1's outlet temperature vs turbine's power generation

6.6. Application in the formation of Carbon Monoxide and Methanol

The captured CO_2 can be used in the formation of carbon monoxide. A simple PFR model is designed and shown in the figure below:

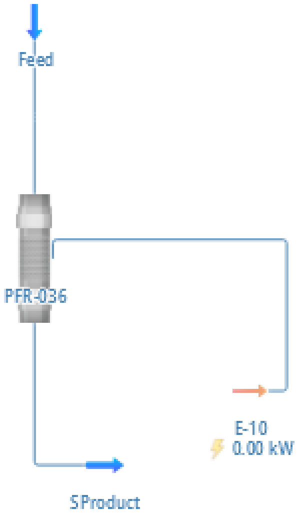


Figure 66: PFR model for formation of carbon monoxide

The following values were used for the PFR model at the ‘Feed’ stream.

Table 65: Feed stream components at PFR model

Methanol	0.00066507361
Water	0.00033065759
Carbon dioxide	0.07073974
Carbon monoxide	0
Hydrogen	0.92826453

The following reaction conditions were described for the PFR model as shown below:

The formation of methanol was described using equation:

$CO_2 + 3H_2 \rightleftharpoons CH_3OH + H_2O$ -49244 kJ/kmol

Reaction rate at base component =

$$\frac{(1.065672664E-13\times(exp(\frac{4811.2}{T}))\times R_1\times R_2)-(41866644.76\times(exp(\frac{-2249.8}{T}))\times P_2\times P_1/(R_2^2))}{(1+(3453.004498*P_2/R_2)+(1.577364283E-3\times(exp(\frac{2068.4}{T}))*(R_2^{0.5}))+(6.628387009E-16*(exp(\frac{14928.9}{T}))\times P_2))^3} \tag{6}$$

The formation of Carbon monoxide takes place as:

$CO_2 + H_2 \rightleftharpoons H_2O + CO$ 41166 kJ/kmol

Reaction rate at base component =

$$\frac{(121.9974326\times(exp(\frac{-11797.5}{T}))\times R_1)-(1.139967781\times(exp(\frac{-7023.5}{T}))\times P_1\times P_2/R_2)}{1+(3453.004498\times\frac{P_2}{R_2})+(1.577364283E-3\times(exp(\frac{2068.4}{T}))\times(R_2^{0.5}))+(6.628387009E-16\times(exp(\frac{14928.9}{T}))\times P_2)} \tag{7}$$

The products obtained at the product stream in vapor phase are as follows:

Table 66 : Mass flow rate of products vapor components

Compounds	Mass flow rate (kg/sec)
Methanol	25865.791
Water	24147.77
Carbon dioxide	121079.54
Carbon monoxide	15472.996
Hydrogen	101967.55

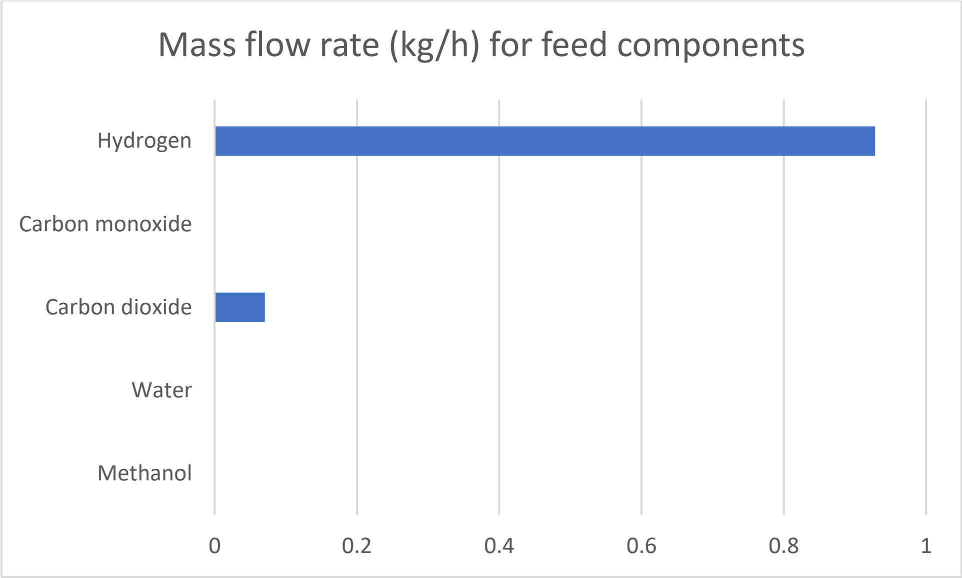


Figure 67: PFR model for formation of carbon monoxide

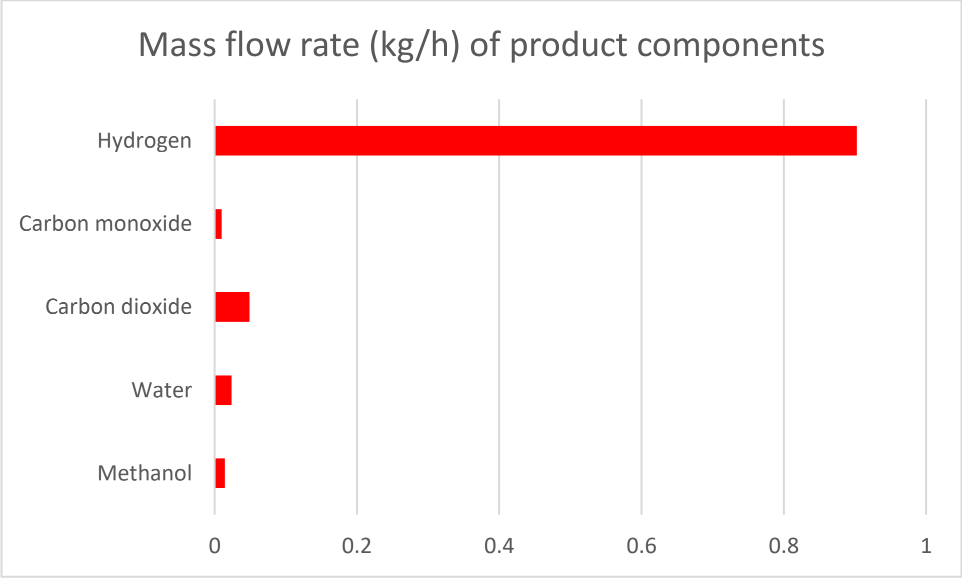


Figure 68: Mass flow rate of product components

6.7. Methane reforming cycle

The methane reforming cycle can be used for the generation of hydrogen using the following reaction: Here, the generated CO_2 can be used for the generation of methane that can form H_2 using the in-built example model provided by the DWSIM development team in the sample section.

Table 67: Mass flow rate of feed components

Feed's compounds	Mass flow rate (kg/hr)
Methane	0.04459
Hydrogen	0
Water	0.050071
Carbon dioxide	0
Carbon monoxide	0

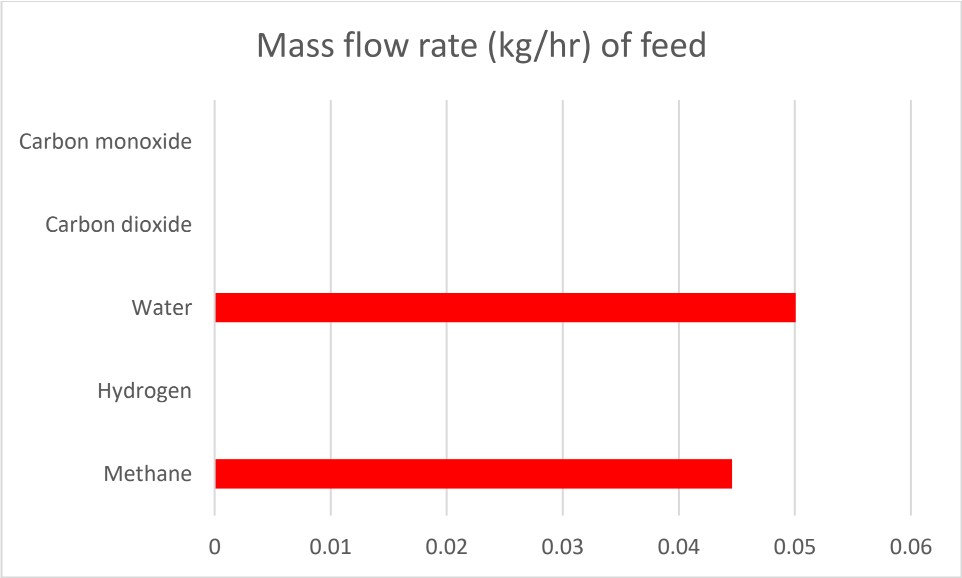


Figure 69: Mass flow rate of product components

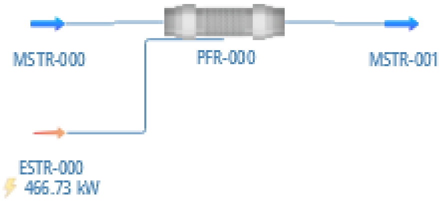


Figure 70: PFR model for methane to H_2 conversion

The reactions that give the product Hydrogen are:

$CH_4 + 2H_2O \rightleftharpoons 4H_2 + CO_2$ 164638.0 kJ/kmol

$CH_4 + H_2O \rightleftharpoons 3H_2 + CO$ 205804.0 kJ/kmol

$H_2O + CO \rightleftharpoons H_2 + CO_2$ -41166.0 kJ/kmol

The mass flow rate of product components in kg/hr is:

Table 68 : Mass flow rate of product's components

Product compounds	Mass flow rate (kg/h)
Methane	0.010814
Hydrogen	0.013182
Water	0.008129
Carbon dioxide	0.009805
Carbon monoxide	0.052731

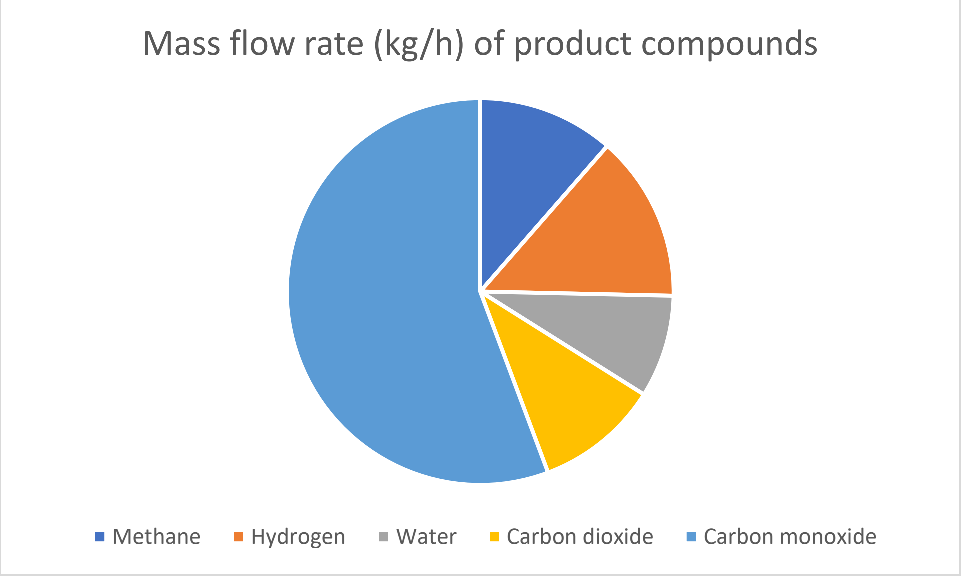


Figure 71: Mass flow rate of product components

6.8. Application in Enhanced Oil Recovery Process

The extractive distillation process can be used for the enhanced oil recovery process, as explained in the abstract that is accessible in **Error! Reference source not found.**. The simulation model made by Ms. Chanchal Attri from the Indian Institute of Technology, Bombay, can be used to determine the feasibility of the removal of carbon dioxide using the cryogenic compression process.

The simulation model accessed from **Error! Reference source not found.** can be utilized to recover impure CO_2 and ethane in the enhanced oil recovery process. The simulation model with the inlet compounds at the 'Feed' stream and mass and heat balance summary at the different equipment and streams is described below:

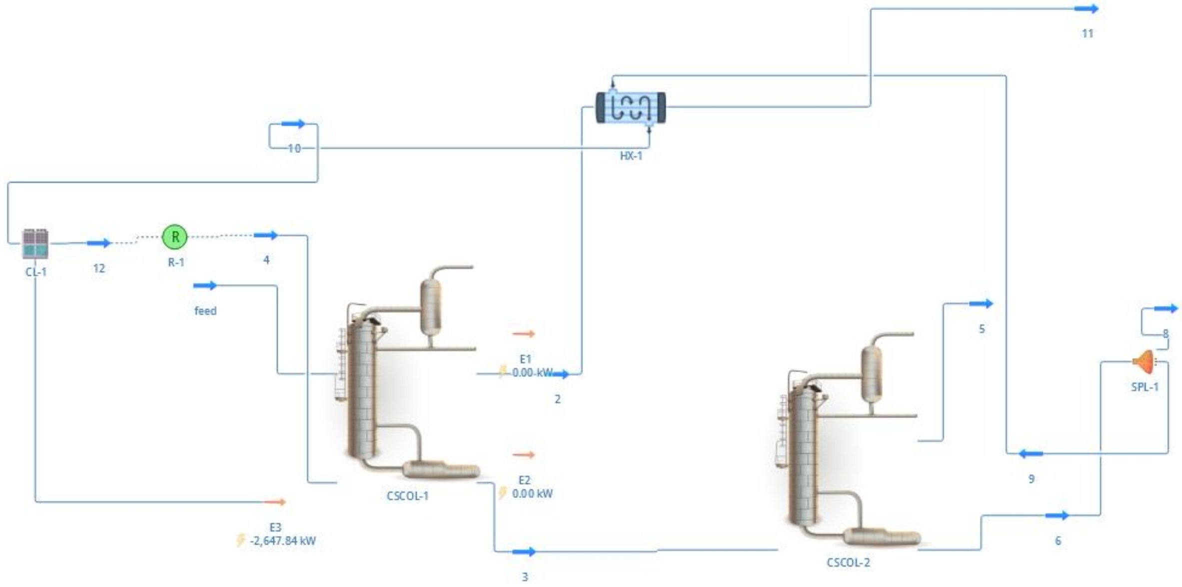


Figure 72: Process simulation model for enhanced oil recovery process

Table 69 : Mass flow rate of fed components

Compounds	Mass flow rate (kg/h)
Ethane	200173.21
Propane	47750.265
Isobutane	63023.064
N-butane	27033.798
Isopentane	22337.262
N-pentane	11324.473
Carbon Dioxide	204381.51

Table 70: Mass and energy balance at different equipment

Equipment	**Type**	**Energy Consumption (-) / Generation (+) (kW)**	**Efficiency (%)**	**MBR (kg/h)**	**EBR (kW)**
CSCOL-1	CAPE-OPEN Unit Operation	47827.2		6.13909E-10	-47827.2
CSCOL-2	CAPE-OPEN Unit Operation	-20251.8		2.35332E-09	20251.8
SPL-1	Stream Splitter	0.0180321		-6.13909E-10	-0.0180321
HX-1	Heat Exchanger	1.61218E-06	91.0473	-2.04636E-10	-1.61218E-06

Equipment	Type	Energy Consumption (-) / Generation (+) (kW)	Efficiency (%)	MBR (kg/h)	EBR (kW)
CL-1	Cooler	-2647.84	100	0	1.66438E-10

Table 71: Mass and energy balance at streams

Name	Mass Flow (kg/h)	Temperature (°C)	Pressure (bar)	Energy Flow (kW)
feed	576024	46.85	25.3313	-773604
2	210910	-12.0688	24.0039	-528835
3	869775	51.4548	24.0039	-647003
4	504662	60.6663	24.0039	-354406
5	196876	-0.0619623	24.0039	-178680
6	672900	101.825	24.0039	-448071
8	168225	101.812	24.0039	-112018
9	504675	101.812	24.0039	-336053
11	210910	68.0428	24.0039	-507838
10	504675	53.85	24.0039	-357050
12	504675	60.7	24.0039	-354402

The results obtained in vapor phase were as follows:

In stream ‘11’:

Table 72: Mass flow rate of different compounds

Compounds (vapor)	Mass flow rate (kg/h)
Ethane	6184.5528
Propane	2515.7041
Isobutane	62.174545
N-butane	5.9539314
Isopentane	0.084512191
N-pentane	0.013739014
Carbon Dioxide	202141.81

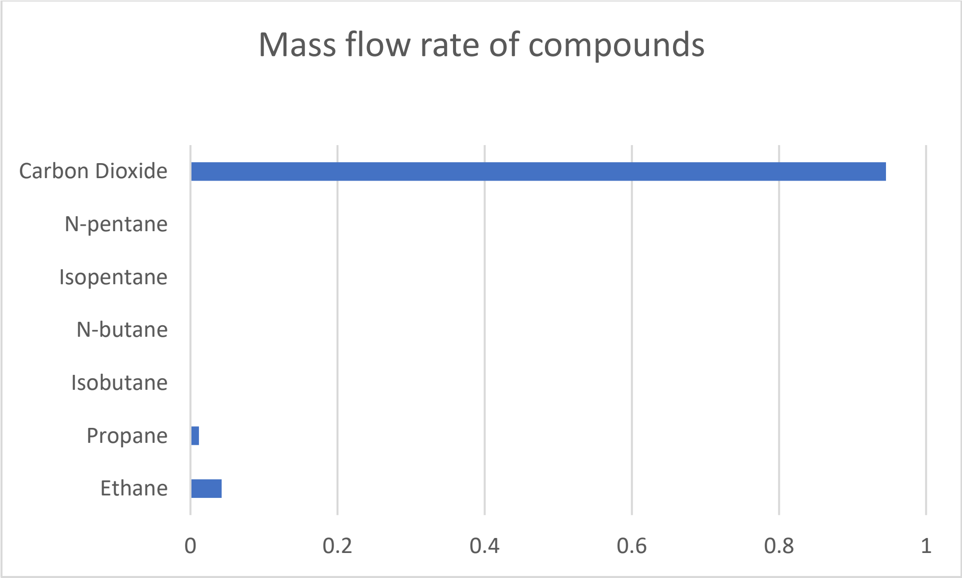


Figure 73: Bar diagram for mass flow rate of different compounds

In stream ‘8’:

Table 73: Mass flow rate of liquid components

Compounds (Liquid)	Mass flow rate (kg/h)
Ethane	0.33622646
Propane	44582.448
Isobutane	62956.794
N-butane	27026.671
Isopentane	22335.042
N-pentane	11323.615
Carbon Dioxide	4.9475464E-08

The above results show that carbon dioxide is not completely free from other compounds, and recovery can be done using cryogenic CO_2 capture technology.

With the addition of a cooler and compressor, as marked in the figure below, a greater amount of impure CO_2 and ethane can be captured, as shown below in Tables 78 and 79:

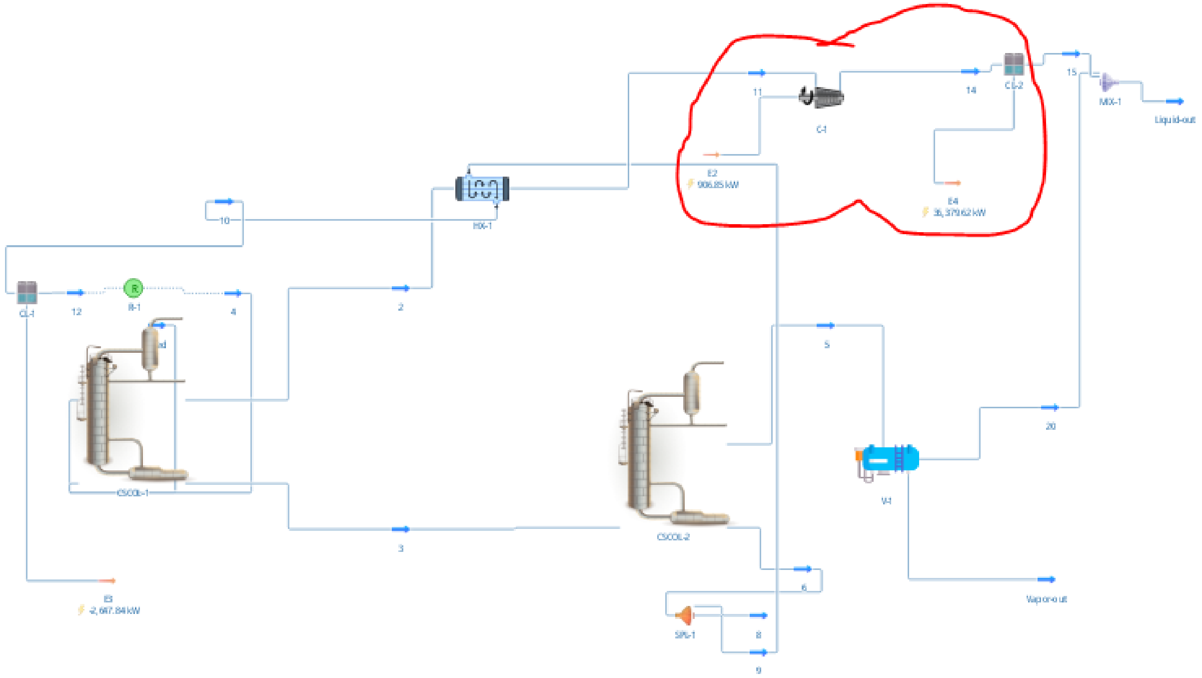


Figure 74: Modified model for enhanced oil recovery process

The mass balance for the overall streams and the equipment used are as follows:

Table 74: Mass and energy balance at different equipment

Equipment	Type	Energy Consumption (-) / Generation (+) (kW)	Efficiency (%)	MBR (kg/h)	EBR (kW)
CSCOL-1	CAPE-OPEN Unit Operation	47646.3		1.84173E-09	-47646.3
C-1	Compressor	-906.852	75	0	3.39829E-08
CSCOL-2	CAPE-OPEN Unit Operation	-20654.3		1.53477E-09	20654.3
SPL-1	Stream Splitter	5.82077E-11		1.02318E-10	-5.82077E-11
HX-1	Heat Exchanger	1.40187E-06	91.9029	0	-1.40187E-06
CL-1	Cooler	-2647.84	100	0	1.05501E-10
CL-2	Cooler	36379.6	100	0	-4.36557E-11
MIX-1	Stream Mixer	-3.1346E-06		0	3.1346E-06
V-1	Gas-Liquid Separator	0.000912764		-5.44965E-05	-0.000912764

Table 75: Mass and energy balance at different streams

Name	Mass Flow (kg/h)	Temperature (˚C)	Pressure (bar)	Energy Flow (kW)
Feed	576024	46.85	25.3313	-773604
2	210910	-12.0688	24.0039	-528662
3	869775	51.4548	24.0039	-646994
4	504662	60.6663	24.0039	-354406
5	196876	-0.0619623	24.0039	-178322
6	672900	101.825	24.0039	-448018
8	168225	101.825	24.0039	-112004
9	504675	101.825	24.0039	-336013
11	210910	71.5219	24.0039	-507626
10	504675	53.85	24.0039	-357050
12	504675	60.7	24.0039	-354402
14	210910	90.1056	29.0039	-506719
15	210910	-150	29.0039	-543099
Liquid-out	403451	-58.5523	24.0039	-717821
Vapor-out	4334.49	-0.0619623	24.0039	-3599.93
20	192541	-0.0619623	24.0039	-174722

Similarly, the products obtained at the liquid-out stream and the vapor-out stream are as follows:

At the liquid-out stream:

Table 76: Mass flow rate of liquid components

Compounds	Mass flow rate (kg/h)
Ethane	195906.9
Propane	3158.0751
Isobutane	62.174599
N-butane	5.9539315
Isopentane	0.084512191
N-pentane	0.013739014
Carbon Dioxide	204318.24

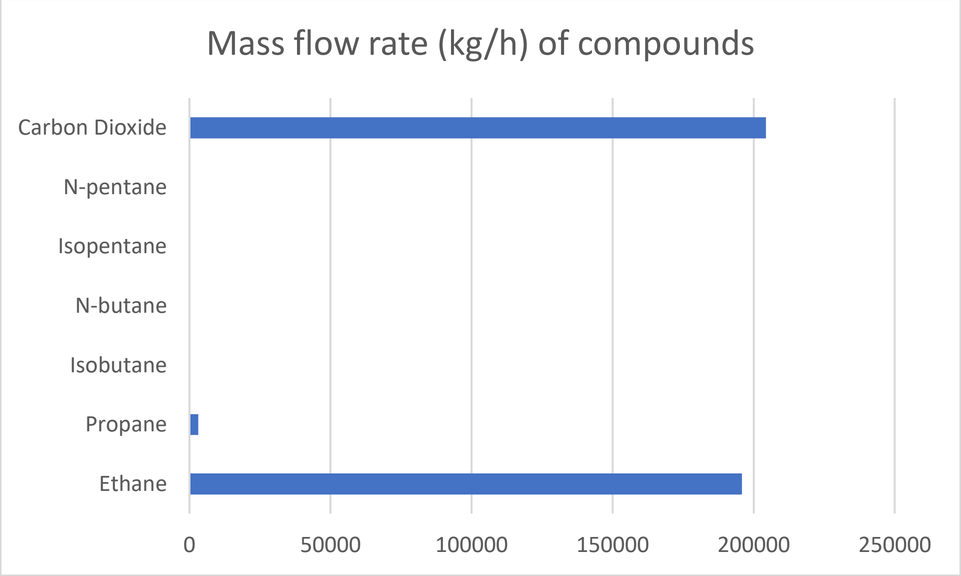


Figure 75: Mass flow rate of compounds at Liquid-out stream

At the Vapor-out stream:

Table 77: Mass flow rate of vapor products

Compounds	Mass flow rate (kg/h)
Ethane	4265.972
Propane	5.241169
Isobutane	1.94E-07
N-butane	3.17E-10
Isopentane	1.12E-17
N-pentane	3.62E-18
Carbon Dioxide	63.27521

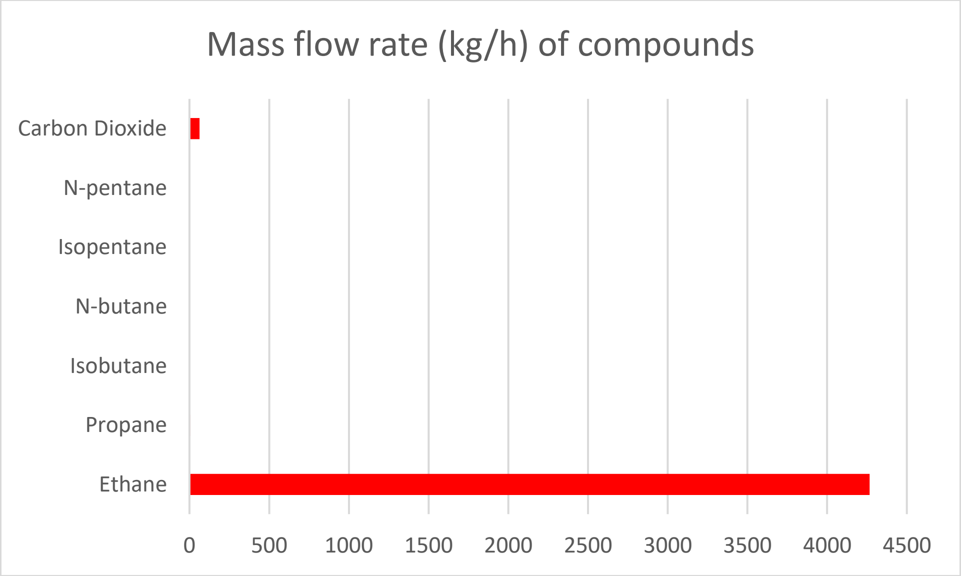


Figure 76: Mass flow rate of compounds at Vapor-out stream

6.9. Formation of urea

Diminishing fossil fuels and global commitments to lowering emissions have emphasized the necessity of exploring modern and sustainable resources to produce urea [41]. CO_2 can be used to produce urea in chemical processing industries by reacting with ammonia. One significant factor contributing to the country's low agricultural output is the very low use of fertilizer, at just 87 kg per hectare of arable land [41][43]. According to the research [34] by Devkota et al., Nepal possesses more than 4 million hectares of cultivable land with a climate that ranges from sub-tropical in the Terai (plains) to temperate in the hilly and lower mountainous regions, providing ideal conditions for a diverse range of agricultural and livestock products. It discusses the urea production capacity of Nepal and determines the amount of ammonia that can be produced in CO_2 capture industries. Gyawali et al., [42] in their research mentioned the production of urea in Nepal, utilizing municipal solid wastes in combination with hydroelectricity which provides solutions to three major problems namely waste management, surplus hydroelectricity utilization, and reduction of urea imports. The urea demand rate in Nepal is notably lower than neighboring countries and major food exporters like India, Bangladesh, and Pakistan, where fertilizer use rates are 175, 319 kg, and 156 kg per hectare of land, respectively [43]. The Green Urea is proposed as new nitrogen-based enhanced efficiency fertilizer (EEF) [44]. Urea can also be used an additive for improving the properties and performance of a biodiesel, such as viscosity, cetane number, oxidative stability, and emissions [45]. Researches have been carried out for using urea as a hydrogen carrier for fuel cell applications. The paper [46] discusses the advantages of urea over other hydrogen carriers, such as high hydrogen density, low cost, easy storage and transportation, and environmental friendliness The problem of heavy dependence on import of fertilizer can be addressed by establishing a fertilizer manufacturing plant. The Snamprogetti process can be used to determine the urea capacity potential of Nepal. The Snamprogetti process's simulation model accessed from [47][48] can be utilized to determine the urea production capacity of Nepal.

The Snamprogetti process for urea manufacture is mostly referred to as "Snamprogetti Urea Technology" or "Snamprogetti Urea Process."

The Snamprogetti Urea Process typically involves the following key steps:

Ammonia Synthesis: Ammonia (NH_3) is the major raw material for urea production. It can be synthesized through the Haber-Bosch process, which involves reacting nitrogen (N_2) and hydrogen (H_2) gases in the presence of a catalyst under high temperature and pressure.

Carbon Dioxide Recovery: Carbon dioxide (CO_2) is another major raw material needed for urea production. It is often obtained from various sources, like power plants, industrial processes, or carbon capture technologies. The CO_2 is recovered, purified, and compressed.

Urea Synthesis: In the urea synthesis step, ammonia and carbon dioxide are reacted in a high-pressure reactor to form urea. This reaction is exothermic and produces ammonium carbamate, which then decomposes to form urea. The process is typically carried out at a pressure of around 150–200 bar and a temperature of about 150–190 °C.

Stripping and Condensation: The urea synthesis reactor effluent contains unreacted ammonia, carbon dioxide, and the desired urea product that forms a mixture, which is then passed through a series of stripper and condenser units to remove the excess ammonia and carbon dioxide and reuse them after the recovery process.

Urea Recovery and Purification: The condensed urea solution is then sent to a series of purification and concentration steps to remove impurities and water, resulting in a high-purity urea product.

Granulation and Prilling: The purified urea solution is typically transformed into solid urea granules or prills, depending on the desired end product. This is achieved by spraying the solution into a fluidized bed granulator or prilling tower, where the urea solidifies as spherical particles.

Cooling and Storage: The urea granules or prills are cooled and then stored in appropriate storage facilities. They are often bagged or bulk-loaded for transportation to end-users or for further processing.

The Snamprogetti Urea Process is known for its efficiency, high purity of the final product, and adaptability to various production capacities, and the technology is widely used in the urea production industry.

The simulation model accessed from [47] can be used for determining the quantity of urea. The model is based on the Snamprogetti Urea Process developed by Mr. Suyash Sunil Sarda from the Indian Institute of Technology, Bombay. The overall description of the processes and reactions used in this simulation model is available in [48].

As mentioned in [34], the daily ammonia production capacity for Nepal for the reaction conditions described in this research article is 1245 tons for 330 days in a year of operation. When 330 tons/day is converted to kg/sec, it is found to be 3.9866 kg/sec as the value of mass flow rate. Using this value as the feed value of the ammonia at feed stream ‘Ammonia Feed (1)’, the value of the mass flow rate of carbon dioxide to be fed is taken from the value of the mass flow rate of CO_2 obtained from our second model proposed for cryogenic CO_2 capture of flue gas, i.e., 14.89 kg/sec of CO_2 as feed into the stream ‘Carbon dioxide (9)’, the value of water’s mass flow rate fed into the stream ‘Wate as 10 kg/sec, oxygen of mole fraction 0.21 at ‘Passivation Air’ and methane’s mass flow rate as 0.666666 kg/sec at ‘Ammonia Feed (1)’ stream, the simulation model’s flowsheet was solved.

As described earlier, using the same reaction conditions as in the model and abstract obtained from [48], the product of urea obtained was found to be 4.6333 kg/sec, which shows that the CO_2 captured from the Sarbottam Cement Industry can be utilized to generate a significant amount of urea.

7. Discussion

CO_2 has become a major threat to the environment and there is a need of development of technology in industrial plants to capture the produced raw or flue gas. Our results showed the cryogenic capture technology is capable to capture both the raw and flue gases. When compared to the cost of the overall process plant for CO_2 capture for the same data of flue gas as in Table 12, the model proposed for two-stage compression in Figure 24 is found to be the least expensive among single, two-stage, and 2-stage cryogenic capture processes. The cost obtained for this 2-stage compression model and membrane-based separation model from [34] shows that the cost of building a membrane-based separation process is less expensive than it but has lower capture efficiency for the same data in Table 12. The capital cost (CAPEX) of capturing by membrane-based separation process discussed in [34] is found to be $10,236,263 for the year 2020, and OPEX is found to be $21,489,733/year and the cost of building a two-stage compression cryogenic process plant shown in Figure 24 is $91,762,163.10, and for the year 2023, OPEX is $40,107,879.66/year. Although the cost of the plant is high, the two-stage model in Figure 24 can be utilized to capture CO_2 with very high purity compared to the membrane separation process. In the research [34], the process generates CO_2 purity of 96.6 mol%, whereas the cryogenic compression models we proposed in this project generate CO_2 of more than 99.6% purity. So, in the case where CO_2 of very high purity is needed, the cryogenic CO_2 process is applicable. The overall analysis shows that the proposed models for CO_2 capture are capable of capturing a high quantity of CO_2, but in practical terms, we can expect the plant to capture more than 90% of CO_2, which is a major efficiency improvement from the perspective of the CO_2 capture system.

Cost reduction methods, like the utilization of the Organic Rankine Cycle (ORC), can be applied to convert the generated heat from coolers used in the process operation to regenerate electricity. The utilization of ORC with the proper selection of organic compounds to operate the process in the plant can reduce the expense of electricity.

8. Conclusion

Through this report of research project, it can be concluded that the proposed models and technologies discussed in the document have the potential to capture and reduce CO_2 emissions in various industries if further researched and implemented. The report highlights the feasibility and sustainability of different methods such as CO_2 capture in the liquid phase, cryogenic CO_2 capture, and waste-to-energy processes. These methods can contribute to reducing greenhouse gas emissions and achieving sustainable development goals. However, it is important to consider the high costs associated with these technologies and the need for further research and development to optimize their efficiency and economic viability.

9. References

[1] H. Ritchie and M. Roser, “Global inequalities in CO2 emissions,” Our World in Data, 2023. [Online]. Available: https://ourworldindata.org/co2-inequality. [Accessed: 17-Sep-2023]. https://www.iea.org/reports/global-energy-review-2021/co2-emissions

[2] International Energy Agency. (2023, March). CO2 Emissions in 2022 [Online]. Available: https://www.iea.org/reports/co2-emissions-in-2022

[3] United States Environmental Protection Agency. (2021, April 13). Sources of Greenhouse Gas Emissions [Online]. Available: https://www.epa.gov/ghgemissions/sources-greenhouse-gas-emissions

[4] What's Your Impact? (n.d.). Carbon Dioxide Emissions [Online]. Available: https://whatsyourimpact.org/greenhouse-gases/carbon-dioxide-emissions

[5] United States Environmental Protection Agency. (2021, April 13). Global Greenhouse Gas Emissions Data [Online]. Available: https://www.epa.gov/ghgemissions/global-greenhouse-gas-emissions-data

[6] R. W. Howarth, "A bridge to nowhere: methane emissions and the greenhouse gas footprint of natural gas," Energy Sci. Eng., vol. 2, no. 2, pp. 47-60, Jun. 2014, doi: 10.1002/ese3.35.

[7] International Energy Agency, "Carbon Capture and Storage - Energy System," IEA, 2021. [Online]. Available: https://www.iea.org/energy-system/carbon-capture-utilisation-and-storage. [Accessed: 17-Sep-2023].

[8] A. K. Mishra, "Making it easier to capture carbon dioxide in the cement industry," Phys.org, 18-Dec-2018. [Online]. Available: https://phys.org/news/2018-12-easier-capture-carbon-dioxide-cement.html. [Accessed: 17-Sep-2023].

[9] MIT Climate Portal, "Carbon Capture," MIT Climate Portal, 2021. [Online]. Available: https://climate.mit.edu/explainers/carbon-capture. [Accessed: 17-Sep-2023].

[10] Global Climate Change, "Greenhouse Gas Emissions Factsheet: Nepal," Global Climate Change, 2017. [Online]. Available: https://www.climatelinks.org/resources/greenhouse-gas-emissions-factsheet-nepal. [Accessed: 17-Sep-2023].

[11] UNFCCC, "Nepal's Long-term Strategy for Net-zero Emissions," UNFCCC, 2020. [Online]. Available: https://unfccc.int/sites/default/files/resource/NepalLTLEDS.pdf. [Accessed: 17-Sep-2023].

[12] National Grid Group, "What is carbon capture and storage?," National Grid Group, 2021. [Online]. Available: https://www.nationalgrid.com/stories/energy-explained/what-is-ccs-how-does-it-work. [Accessed: 17-Sep-2023].

[13] MIT Climate Portal, "Carbon Capture," MIT Climate Portal, 2021. [Online]. Available: https://climate.mit.edu/explainers/carbon-capture. [Accessed: 17-Sep-2023].

[14] N. Sakkal and J. Byrne, "What is carbon capture and how does it fight climate change?," ABC News, 23-Jan-2021. [Online]. Available: https://www.abc.net.au/news/science/2021-01-23/green-hydrogen-renewable-energy-climate-emissions-explainer/13081872. [Accessed: 17-Sep-2023].

[15] J. Johnson, "What Are the Uses of Carbon Dioxide Gas?," Sciencing, 02-Apr-2018. [Online]. Available: https://sciencing.com/uses-carbon-dioxide-gas-6364016.html. [Accessed: 17-Sep-2023].

[16] Vedantu, "Uses of Carbon Dioxide - Learn Important Terms and Concepts," Vedantu, 2020. [Online]. Available: https://www.vedantu.com/evs/uses-of-carbon-dioxide. [Accessed: 17-Sep-2023].

[17] Royal Society, “Ammonia: zero-carbon fertiliser, fuel and energy store,” Royal Society, 2018. [Online]. Available: https://royalsociety.org/-/media/policy/projects/green-ammonia/green-ammonia-policy-briefing.pdf. [Accessed: 17-Sep-2023].

[18] Methanol Institute, “What is Methanol, its uses, energies,” Methanol Institute, 2021. [Online]. Available: https://www.methanol.org/. [Accessed: 17-Sep-2023].

[19] Mitsubishi Gas Chemical Company Inc., “The Many Uses of Methanol,” Mitsubishi Gas Chemical Company Inc., 2019. [Online]. Available: https://www.mgc.co.jp/eng/rd/technology/methanol.html. [Accessed: 17-Sep-2023].

[20] World Economic Forum, “Hydrogen from hydropower could hold the key to unlocking renewable energy,” World Economic Forum, 28-Jul-2020. [Online]. Available: https://www.weforum.org/agenda/2020/07/hydrogen-hydropower-renewable-energy/. [Accessed: 17-Sep-2023].

[21] UNFCCC, “Nepal’s Long-term Strategy for Net-zero Emissions,” UNFCCC, 2020. [Online]. Available: https://unfccc.int/sites/default/files/resource/NepalLTLEDS.pdf. [Accessed: 17-Sep-2023].

[22] World Economic Forum, “Hydrogen from hydropower could hold the key to unlocking renewable energy,” World Economic Forum, 28-Jul-2020. [Online]. Available: https://www.weforum.org/agenda/2020/07/hydrogen-hydropower-renewable-energy/. [Accessed: 17-Sep-2023].

[23] The Current, “Plastic’s Carbon Footprint,” The Current, 04-Feb-2019. [Online]. Available: https://news.ucsb.edu/2019/019424/plastics-carbon-footprint. [Accessed: 17-Sep-2023].

[24] OECD Environment Directorate, “Plastic leakage and greenhouse gas emissions are increasing,” OECD Environment Directorate, 2020. [Online]. Available: https://www.oecd.org/environment/plastics/increased-plastic-leakage-and-greenhouse-gas-emissions.htm. [Accessed: 17-Sep-2023].

[25] A. K. Singh et al., “The clean energy aspect of plastic waste — hydrogen gas production, CO_2 reforming, and plastic waste management coincide with catalytic pyrolysis — an extensive review,” Environmental Science and Pollution Research, vol. 28, no. 8, pp. 8697–8724, Feb. 2021. [Online]. Available: https://link.springer.com/article/10.1007/s11356-023-26908-3. [Accessed: 17-Sep-2023].

[26] S. Devkota, R. Pokhrel, B. Rayamajhi, and B. Uprety, “Design and cost estimation of a CO2 capture plant from cement flue gas for urea production in Nepal,” Int. J. Greenhouse Gas Control, vol. 111, p. 103484, Sep. 2021, doi: 10.1016/j.ijggc.2021.103484.

[27] Chaudhary, Y., Gautam, S., Poudyal, A. R., Joshi, R., & Uprety, B. (2022). Review on the Different Processes of Urea Production for Achieving Sustainable Development Goals in Nepal. *Journal of Institute of Science and Technology*, *27*(1), 69-81.

[28] Adhikari, A., Arachchige, U. S. P., Melaaen, M. C., Dotel, U. R., & Pokhrel, R. (2014, March). Role of solar flat plate collectors in reducing green house gases in Nepal. In *2014 5th International Renewable Energy Congress (IREC)* (pp. 1-4). IEEE.

[29] G. B. Khadka, R. A. Mandal, and A. B. Mathema, “Comparison Growing Stock, Carbon Stock and Biodiversity in and Around Banke National Park, Nepal,” Int. J. Bot., vol. 5, no. 3, pp. 21-26, 2019.

[30] K. C. Anup, G. Bhandari, G. R. Joshi, and S. Aryal, “Climate change mitigation potential from carbon sequestration of community forest in mid hill region of Nepal,” Int. J. Environ. Prot., vol. 3, no. 7, p. 33, 2013.

[31] M. S. K. Sarkar, A. Takemoto, S. Sadeka, M. M. Islam, and A. Q. Al-Amin, “Achieving Sustainable Development Goals (SDGs) among the South Asian Countries: Progress and Challenges,” Int. J. Reg. Dev., vol. 9, no. 2, pp. 42-61, 2022.

[32] R. Vineel and S. Dixit, “Control Global Warming by Reducing Atmospheric CO2 to Carbon and Producing Energy,” Hydro Nepal: J. Water, Energy Environ., vol. 6, pp. 38-41, 2010.

[33] Gyawali, E. P. Advance in Environmental Waste Management & Recycling.

[34] S. Devkota, S. Ban, R. Shrestha, and B. Uprety, “Techno-economic analysis of hydropower based green ammonia plant for urea production in Nepal,” Int. J. Hydrogen Energy, 2023, in press, doi: 10.1016/j.ijhydene.2023.01.123.

[35] A. Takashina et al., “Development of a novel flue gas treatment system for CO2 capture and utilization,” Energy Procedia, vol. 63, pp. 1419-1426, 2014, doi: 10.1016/j.egypro.2014.11.152.

[36] Indiamart.com, "Liquid CO2 Storage Tank," Indiamart InterMESH Limited, 2023. [Online]. Available: https://www.indiamart.com/proddetail/liquid-co2-storage-tank-25517701797.html. [Accessed: Oct 1, 2023].

[37] “Inflation rates in Nepal - Worlddata.info,” [Online]. Available: https://www.worlddata.info/asia/nepal/inflation-rates.php. [Accessed: Oct. 2, 2023].

[38] International Trade Administration. [Online]. Available: https://www.trade.gov/country-commercial-guides/nepal-import-tariffs. [Accessed: Oct. 2, 2023].

[39] Privacy Shield. [Online]. Available: https://www.privacyshield.gov/ps/article?id=Nepal-Import-Tariffs. [Accessed: Oct. 2, 2023].

[40] FOSSEE. “Flowsheeting Project | DWSIM Flowsheeting Project”. [Online]. Available: https://dwsim.fossee.in/flowsheeting-project/dwsim-flowsheet-run/1045. [Accessed: 11-Oct-2023].

[41] L. Sun and R. Smith, “Rectisol wash process simulation and analysis,” J. Clean. Prod., vol. 39, pp. 321-328, Jan. 2013, doi: 10.1016/j.jclepro.2012.05.049.

[42] K. Gyanwali, S. Karki, P. Adhikari, S. Devkota, and P. Aryal, “Techno-economic assessment of green urea production utilizing municipal solid waste and hydropower in Nepal,” in J. Cleaner Prod., vol. 419, 138320, Jun. 2023, doi: 10.1016/j.jclepro.2023.138320.

[43] Y. Chaudhary, S. Gautam, A. R. Poudyal, R. Joshi, and B. Uprety, “Review on the different processes of urea production for achieving sustainable development goals in Nepal,” J. Inst. Sci. Technol., vol. 27, pp. 69-81, 2022, doi: 10.3126/JIST.V27I1.45515.

[44] N. Yahya and N. Yahya, “Urea fertilizer: The global challenges and their impact to our sustainability,” in Green Urea: For Future Sustainability, Singapore: Springer, 2018, pp. 1-21, doi: 10.1007/978-981-10-7871-2_1.

[45] A. K. Singh, S. K. Singh, and R. K. Singh, “Urea as a potential additive for enhancing the performance of biodiesel: A review,” Renew. Sustain. Energy Rev., vol. 82, pp. 3134-3146, Feb. 2018, doi: 10.1016/j.rser.2017.10.039.

[46] Y. Chaudhary, S. Gautam, A. R. Poudyal, R. Joshi, and B. Uprety, “Review on the different processes of urea production for achieving sustainable development goals in Nepal,” J. Inst. Sci. Technol., vol. 27, pp. 69-81, 2022, doi: 10.3126/JIST.V27I1.45515.

[47] FOSSEE. “DWSIM Flowsheet Run.” DWSIM Flowsheeting Project. [Online]. Available: https://dwsim.fossee.in/flowsheeting-project/dwsim-flowsheet-run/342. [Accessed: Oct. 14, 2023].

[48] FOSSEE. “Full Download Project.” DWSIM Flowsheeting Project. [Online]. Available: https://dwsim.fossee.in/flowsheeting-project/full-download/project/342. [Accessed: Oct. 14, 2023].