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CO₂ Capture and Conversion to Methanol with EEMPA

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CO2 Capture and Conversion to Methanol with EEMPA

Abstract

Increasing amounts of carbon dioxide (CO₂) in the atmosphere has been a primary contributor to the changing climate is having disastrous impacts on our planet and its inhabitants. Creating new strategies to combat the ongoing climate crisis has gained significant momentum in recent years with the efforts to slow and reverse climate change. Of these promising new technologies, the implementation of carbon capture and utilization (CCU) has been recognized to have a high potential by taking in CO₂ emitted from point sources and using it to produce a value-added product. With a wide range of methanol uses and large amounts of CO₂ emitted during the typical process of industrial methanol production, methanol is an attractive product for production through CCU.

Through the proposed process, a water-lean binding organic liquid, N-(2-ethoxyethyl)-3-morpholinopropan-1-amine (EEMPA), is used to capture CO₂ emitted in the flue gas of a coal fired power plant through an integrated capture and conversion process. The process begins with an absorption column to remove CO₂ from the flue gas by absorption to EEMPA. The bound CO₂ then undergoes a hydrogenation reaction to desorb CO₂ from EEMPA and to produce methanol. In the final stages of the process, the mixture undergoes a series of separations to recycle EEMPA back to the absorption column, to recycle the excess hydrogen back to the hydrogenation reaction, and to isolate the desired methanol product with a mass purity of 99.6%.

The proposed project was found to be carbon negative and pairing it with an aggressive carbon tax, influenced by the precedent set by other countries, or charging a green premium indicates that the process has the potential to become profitable. Currently, the project's return on investment stands at 19.33%, the internal rate of return at 21.97%, and the net present value is \$3,734,600.

Disciplines

Biochemical and Biomolecular Engineering | Chemical Engineering | Engineering



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Philadelphia, PA 19104

April 20th, 2021

Dear Professor Bruce Vrana, Professor Talid Sinno, and Dr. Matthew Targett,

The following report contains the complete design for the process of carbon dioxide (CO₂) capture and conversion to methanol with N-(2-ethoxyethyl)-3-morpholinopropan-1-amine (EEMPA). Our process will have the capacity to produce 2,639 tons/year of methanol with 99.6% mass purity. Utilizing carbon captured from the emissions of coal fired power plants, this carbon negative process will help to reduce global CO₂ emissions, assisting on the path towards a solution to the climate emergency. The realization of this process will begin with the absorption of CO₂ to the binding organic liquid EEMPA, followed by a hydrogenation reaction to desorb the CO₂ from EEMPA and to produce methanol. The final stages of the process include several refining steps to separate EEMPA for recycle and methanol for distribution.

Economic and profitability analysis of this process conclude that the return on investment will be 19.33%, the internal rate of return 21.97%, and the net present value is \$3,734,600. Pairing the proposed process with an aggressive carbon tax or the charge of a green premium indicates that the project has the potential for profit.

We would like to sincerely thank you both for all of your help and support throughout the semester. We greatly appreciate the abundance of insight and guidance provided on our project and as always, we look forward to receiving your feedback.

Sincerely,

Yatin Arora

Ashwin Koul

Melissa Tanaka

CO₂ Capture and Conversion to Methanol with EEMPA

Yatin Arora

Ashwin Koul

Melissa Tanaka

Proposed by Dr. Matthew Targett

Project Advisor: Dr. Talid Sinno

University of Pennsylvania School of Engineering and Applied Sciences

Department of Chemical and Biomolecular Engineering

April 20, 2021

Table of Contents

1. Abstract	5
2. Introduction and Objective	6
2.1. Background	6
2.2. Motivations and Goals	9
2.3. Time Chart	11
3. Innovation Map	12
4. Market and Competitive Assessment	13
5. Customer Requirements	15
6. CTQ Variables - Product Requirements	16
7. Product Concepts	17
8. Superior Product Concepts	18
9. Competitive Patent Analysis	19
10. Preliminary Process Synthesis	21
10.1 BOL Selection	21
10.2 Flue Gas	21
10.3 Absorber	22
10.4 BOL Refining	25
11. Assembly of Database	28
12. Block Flow Diagram	30
13. Process Flow Diagram	31
13.1 Equipment Identifiers and Descriptions	32
14. Material Balances	33
15. Process Descriptions	39
15.1 Flue Gas Feed	39
15.2 CO ₂ Absorption to BOL	39
15.3 Hydrogenation of Bound CO ₂ to Methanol	41
15.4 BOL Refining and Methanol Separation	42
15.5 Hydrogen Recycle	44
15.6 BOL Recycle	45

16. Energy Balance and Utility Requirements	46
17. Equipment List and Unit Descriptions	48
17.1 Condensers	48
17.2 Blowers	48
17.3 Absorption Tower	51
17.4 Pumps	52
17.5 Hydrogenation Reactor	53
17.6 Flash Vessel	54
17.7 Distillation Towers - BOL Separation	54
18. Specification Sheets	56
19. Equipment Cost Summary	80
20. Fixed Capital Investment Summary	82
21. Operating Costs - Costs of Manufacture	83
22. Other Important Considerations	86
22.1 Location	86
22.2 Environmental Factors	88
22.3 Public and Employee Safety, Health, and Welfare	91
22.4 Global, Cultural, Societal, and Ethical Factors	94
22. Profitability Analysis	96
23. Conclusions and Recommendations	99
24. Acknowledgements	100
25. Bibliography	101
26. Appendix A: Miscellaneous Calculations	105
27. Appendix B: Vendor Specification Sheets	138
28. Appendix C: Patents	140
30. Appendix D: Material Safety Data Sheets	141

1. Abstract

Increasing amounts of carbon dioxide (CO₂) in the atmosphere has been a primary contributor to the changing climate is having disastrous impacts on our planet and its inhabitants. Creating new strategies to combat the ongoing climate crisis has gained significant momentum in recent years with the efforts to slow and reverse climate change. Of these promising new technologies, the implementation of carbon capture and utilization (CCU) has been recognized to have a high potential by taking in CO₂ emitted from point sources and using it to produce a value-added product. With a wide range of methanol uses and large amounts of CO₂ emitted during the typical process of industrial methanol production, methanol is an attractive product for production through CCU.

Through the proposed process, a water-lean binding organic liquid, N-(2-ethoxyethyl)-3-morpholinopropan-1-amine (EEMPA), is used to capture CO₂ emitted in the flue gas of a coal fired power plant through an integrated capture and conversion process. The process begins with an absorption column to remove CO₂ from the flue gas by absorption to EEMPA. The bound CO₂ then undergoes a hydrogenation reaction to desorb CO₂ from EEMPA and to produce methanol. In the final stages of the process, the mixture undergoes a series of separations to recycle EEMPA back to the absorption column, to recycle the excess hydrogen back to the hydrogenation reaction, and to isolate the desired methanol product with a mass purity of 99.6%.

The proposed project was found to be carbon negative and pairing it with an aggressive carbon tax, influenced by the precedent set by other countries, or charging a green premium indicates that the process has the potential to become profitable. Currently, the project's return on investment stands at 19.33%, the internal rate of return at 21.97%, and the net present value is \$3,734,600.

2. Introduction and Objective

2.1. Background

Fossil fuels have been heavily relied upon in the United States and other parts of the globe since the beginning of the Industrial Revolution around the 1760s. While fossil fuels helped launch the modernization of our world, the large quantity of greenhouse gases emitted from these sources has increasingly become a problem for our planet's prosperity. Accumulating amounts of greenhouse gases in the atmosphere have contributed heavily to climate change which has caused large shifts in weather patterns around the globe since the mid-20th century. With abnormally high levels of greenhouse gases in the atmosphere, incoming solar radiation gets trapped against the surface of the Earth and the heat is not allowed to escape (NASA, 2021). Climate change has been proven to result in disastrous effects such as sea level rise, as well as increasing hurricane, drought, and wildfire intensity. For the health and safety of all of our present and future communities, actions to fight the climate emergency must be taken, and an effort to reduce greenhouse gas emissions must be made a priority.

In 2018, CO₂ made up about 81% of greenhouse gas emissions and is considered to be the primary emission sourced from human activity (EPA, n.d.). CO₂ is a chemical compound that is naturally released through processes such as volcanic eruptions and respiration (NASA, 2021), however, during the years spanning 2000 through 2014, anthropogenic CO₂ emissions increased an average of 2.6% per year, which was much greater than the 1.72% increase seen between 1970 and 2000 (Mac Dowell et al., 2017). For this reason, reducing CO₂ emissions is often a central focus for climate change mitigation strategies.

Typically, methanol is produced industrially through natural gas reforming which has been estimated to emit 0.54 tons of CO₂/ton of methanol produced (Methanol Fuels, n.d.). Although the

amount of CO₂ emitted has declined significantly over the last ten years due to greater efficiencies in new technologies, methanol production and its associated CO₂ emissions remains a large contributor to the climate crisis.

Carbon capture and sequestration (CCS) has emerged as a promising new technology to be coupled with the reduction in fossil fuel use in the effort to slow and reverse climate change. However, high costs associated with CCS bring about many difficulties in its effectiveness and the feasibility of its implementation. To lessen the burden of high costs associated with CCS, carbon capture and utilization (CCU) is a promising potential solution. In CCU, the captured CO₂ is used to produce a wide variety of value-added products, as shown in Figure 2.1 below (Targett, n.d.).

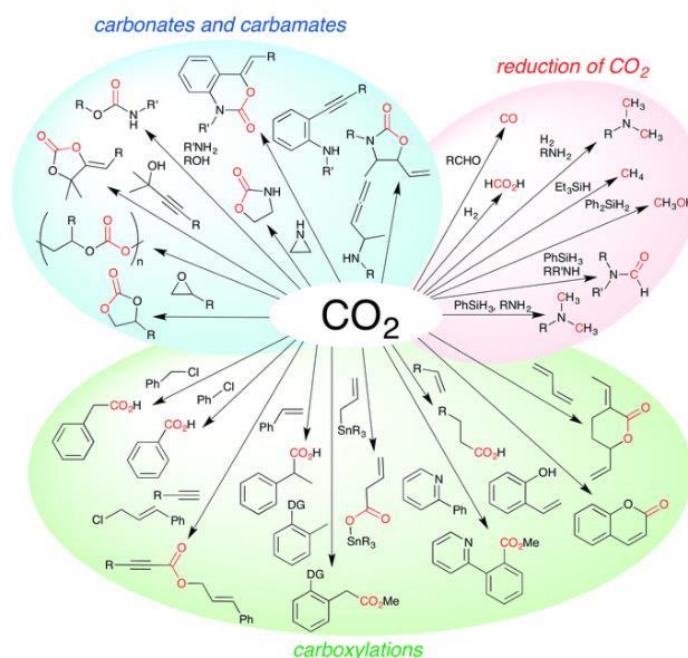


Figure 2.1. Visual representation of the numerous possibilities for products that can be synthesized by captured CO₂.

Carbon capture is best accomplished with aqueous amine-based absorption because of the effective reversible reactions between amines and CO₂ (Dutcher et al., 2015). To reduce the energy and capital costs associated with CCU projects, use of water-lean solvents have been suggested as

they have been shown to decrease the required solvent recirculation and water condensation and vaporization (Jaing et al., 2021).

2.2. Motivations and Goals

To avoid the disastrous effects of climate change, CO₂ emissions need to be reduced and carbon capture is one of the most promising means to achieve this reality. Due to the high costs and energy demands incurred by CCS, a more practical strategy to effectively reduce CO₂ emissions is CCU. Methanol production involves large quantities of CO₂ emissions, so producing it with captured CO₂ will greatly decrease the emissions involved in its synthesis. Methanol is of particularly high interest because it is already produced in high volumes and is used as a raw material to create many chemicals and products, or directly as a fuel.

This project aims to demonstrate the feasibility of decreasing the amount of CO₂ emitted by methanol production by incorporating it into CCU. By using the CO₂ generated by coal fired power plants, we hope to minimize the overall net CO₂ emissions totaled from both processes. Research at the US Department of Energy's Pacific Northwest National Laboratory (PNNL) has indicated the potential for success at capturing and converting CO₂ to methanol through an integrated capture and conversion process. The goal is to find the optimal commercial process to capture and convert CO₂ from coal fired plant flue gas sources into methanol.

The process will be designed for a capacity of 100 TPD of CO₂ captured and the goal is to produce methanol with 99.6% purity. The process inputs are CO₂ from flue gas, H₂, binding organic liquid (BOL), and catalyst, with the hydrogen being fed at a ratio that is slightly above stoichiometric in order to shift the equilibrium in favor of CO₂ conversion (Targett, n.d.). We aim to conduct a successful techno-economic evaluation with an accurate process model and design of the main process steps: absorption, hydrogenation, BOL refining, and solvent recycle. Through our model, we hope to find the Opex cost, Capex investment, and IRR/NPV. The financial success of our project will take into consideration tax credits for CO₂ utilization, and if the process is not

found to produce a profit, we aim to complete a sensitivity analysis to determine what factors can be altered to make the project profitable (Targett, n.d.).

2.3. Time Chart

	Description of Milestone	Completion Date	Status
1	Basic Project Research		
1.1	Preliminary background research	December 2020	Complete
1.2	Determine main goals	December 2020	Complete
1.3	Basic block flow diagram	December 2020	Complete
2	Process and Equipment Design		
2.1	Create block flow diagram	January 2021	Complete
2.2	Create process flow diagram	January 2021	Complete
2.3	Select BOL	January 2021	Complete
2.4	Complete material balances	February 2021	Complete
2.5	Complete energy balances	February 2021	Complete
2.6	Choose plant location	February 2021	Complete
2.7	Process simulation in ASPEN	March 2021	Complete
2.8	Utilities requirements	March 2021	Complete
2.9	Detailed equipment design	March 2021	Complete
2.1	Heat Integration	March 2021	Complete
3	Economic Evaluations		
3.1	Equipment and materials costing	March 2021	Complete
3.2	Profitability analysis	March 2021	Complete
3.3	Startup costs	March 2021	Complete
3.4	Operation costs	March 2021	Complete
4	Health, Safety, and Environmental Evaluations		
4.1	Safety analysis	April 2021	Complete
4.2	Research environmental considerations	April 2021	Complete
4.3	Determine potential health impacts	April 2021	Complete
4.4	Analyze global, cultural, and societal factors	April 2021	Complete
5	Report and Presentation		
5.1	Written report due to faculty advisor	April 13, 2021	Complete
5.2	Revised written report due to Professor Vrana	April 20, 2021	Complete
5.3	Design presentation	April 27, 2021	

Figure 2.2. Objective-Time Chart for the completion of CO₂ capture and conversion to methanol with EEMPA design

3. Innovation Map

N/A

4. Market and Competitive Assessment

There are a variety of possible products that can be made from captured CO₂. However, methanol is a highly attractive option and will be produced by the proposed process. Methanol can be directly used as a fuel source and is an effective hydrogen carrier because it can generate H₂ on demand at low temperatures. Additionally, methanol can be used as a raw material to make many commonly used and produced chemical products such as formaldehyde, dimethyl ether, light olefins, and gasoline (Targett, n.d.), with about 40% of all methanol consumption going towards energy applications as of 2015 (Methanol Institute, 2021).

Some of the largest United States methanol manufacturers include Celanese Corporation, Caribbean Gas Chemical, US Methanol, Natgasoline LLC, and Valero Energy Corp. Methanex is currently the largest methanol producer and supplier in North America as well as in Asia Pacific, Europe and South America. As well as selling methanol produced at Methanex facilities, Methanex purchases agreements with outside suppliers to buy methanol. Methanex produces methanol with a purity of 99.85% (Methanex, 2021) leaving an opening in the market for our methanol which will be produced as a bulk commodity chemical with a purity of 99.6%, making it ideal for use in laboratory settings (Millipore Sigma, 2021).

Globally, methanol is already being produced at a rate of 100 billion liters annually (Targett, n.d.). In North America, methanol costs USD 492/MT at the Methanex non-discounted reference price (Methanex, 2021). Due to its large size and demand, the methanol industry generates \$55 billion in economic activity annually, creating over 90,000 jobs around the globe (Methanol Institute, 2021). The worldwide production capacity in 2019 was approximately 148 million metric tons, with 5.2 million metric tons of methanol being produced in the United States in 2018. This global production rate is expected to increase greatly by the year 2030 to about 311

million metric tons due to the large number of planned methanol plants around the world (Garside, 2020). As of 2018, the leader in methanol production was the Asia Pacific region, responsible for about 61.6% of overall methanol revenue. Within the Asia Pacific region, China plays a significant role in the methanol market, producing 75% of the region's methanol, as well consuming the most methanol fuel (Grand View Research, 2019).

5. Customer Requirements

Methanol is most commonly used as a clean energy source and is a base component for many everyday products and applications (Methanex, 2021). The market for methanol production largely focuses on long term contracts or partnerships between customers and manufacturers (Grand View Research, 2019). Within our process, methanol will be produced as a bulk commodity chemical in the liquid form with a 99.6% purity, allowing for consistent consumer-producer relations to hold over the long term.

As of 2018, about 24.3% of the total volume of methanol produced went towards the production of formaldehyde. Formaldehyde resins are mainly used to increase fuel efficiency or to mitigate bacterial growth and the spread of pathogens (Grand View Research, 2019). Formaldehyde is commonly used to produce adhesives, molding materials, and pesticides, and is a large part of the growing construction, automobile, and textile industries (Fortune Business Insights, 2020).

With the widespread recognition of the climate emergency and other environmental concerns, the demand for methanol is expected to increase due to the desire for greener fuel alternatives (Fortune Business Insights, 2020).

6. CTQ Variables - Product Requirements

N/A

7. Product Concepts

N/A

8. Superior Product Concepts

N/A

9. Competitive Patent Analysis

As of 2020, the global market for carbon capture, utilization, and storage was valued at 1.6 billion USD, and this number is predicted to grow to 3.5 billion USD by 2025. Europe has the fastest growing carbon capture, utilization, and storage market due to Norway's aggressive strategies for cutting carbon emissions, as well as numerous planned projects in the Netherlands and the UK, notably, Norway Full Chain and Caledonia Clean, respectively (Business wire, 2020). As for the production of methanol with captured CO₂, Breathe Applied Sciences and Carbon Recycling International are global leaders of the market (Cho, 2019).

I. Breathe

Finalists for the 2019 NRG COSIA Carbon XPRIZE, Breathe aims to convert captured CO₂ from coal and natural gas fired power plants into methanol and carbon monoxide with high purity. Their process utilizes a range of copper, zinc, aluminum and iron-based catalysts to reduce methanol production costs by 25% and carbon monoxide costs by 50%. Their revenue is mainly sourced from licensing and it is estimated that subsidies are not needed to make the process profitable. The company is based in India and is mainly playing into the Indian market, however the final process is planned to be geographically unrestrained, to be deployed across the globe (Breathe, 2021).

II. Carbon Recycling International (CRI)

A leader in power-to-methanol technology, CRI produces renewable methanol from CO₂, hydrogen, and electricity. Their process captures CO₂ from geothermal power plants to make hydrogen which is then converted to methanol through a catalytic reaction. The overall process produces very few emissions as most of their electricity is sourced from geothermal and hydro providers. Based in Iceland, the company sells the methanol they have produced as a gasoline

additive and for biodiesel production (Cho, 2019). CRI's standard process design has a production capacity of 50.000-100.000 ton/yr methanol that can be scaled up or down depending on what is required (Carbon Recycling International, 2021).

10. Preliminary Process Synthesis

10.1 BOL Selection

Deciding upon a BOL was essential to the early stages of process design due to the process's heavy dependence on BOL properties. Ethanol was considered as a BOL because it is a well-known compound and much of the preliminary research done by PNNL was accomplished with ethanol as the BOL. Methanol was also considered as a potential BOL because of the convenient recycle stream it would involve.

N-(2-ethoxyethyl)-3-morpholinopropan-1-amine (EEMPA), seen below in Figure 10.1, was ultimately selected as our BOL. EEMPA was deemed to work best with our planned system because our preliminary flowsheet was most compatible with a heavy BOL due to the dependence on mass differences in the final BOL refining steps. Solvent properties and parameters for EEMPA are presented in Table 28.1 in Appendix B.

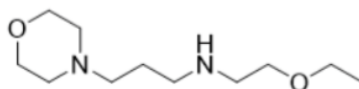


Figure 10.1 Chemical structure of the selected binding organic liquid, N-(2-ethoxyethyl)-3-morpholinopropan-1-amine (EEMPA).

10.2 Flue Gas

The temperature, pressure, and composition of the incoming stream was to be determined from the selected flue gas source. Considering which industries emitted the most CO₂, flue gas from natural gas and coal fired power plants were both considered.

In order to remove some of the excess water entering the process, the flue gas was planned to be cooled prior to entering the absorber. Initially this was suggested to occur with refrigeration, however an alternative was sought out after weighing the high costs and energy requirements

associated with refrigeration. To reduce the amount of water entering the process, the flue gas is pretreated with cooling water to reduce the temperature to 25°C, and then run through a second heat exchanger cooled with chilled water to drop the dew point to 16°C to achieve a steady state of 1.6 wt.% of water in EEMPA and to avoid the formation of a second phase of water.

10.3 Absorber

The goal of the absorber is to capture 90% of CO₂ from flue gas using the binding organic liquid, EEMPA. The absorption column will be driven by pressure differences and managing and minimizing changes in temperature within the column is a main focus. The purpose of the column is to allow CO₂ to absorb to the BOL, EEMPA, shown by the reaction in Equation 1 below.



As the temperature within the column increases, less CO₂ will bind to EEMPA and some of the bound CO₂ may desorb. By minimizing temperature changes, we will be able to produce an efficient absorption column and maximize methanol production by limiting desorption.

The absorption column will be operated at 30°C and a pressure of 1 atm. These operating conditions were chosen based on absorption kinetic data shown in Figure 11.2 to maximize the liquid film mass transfer coefficient and hence, maximize the mass-transfer rate. Figure 10.2 below shows a detailed pictorial representation of the absorber and its associated streams.

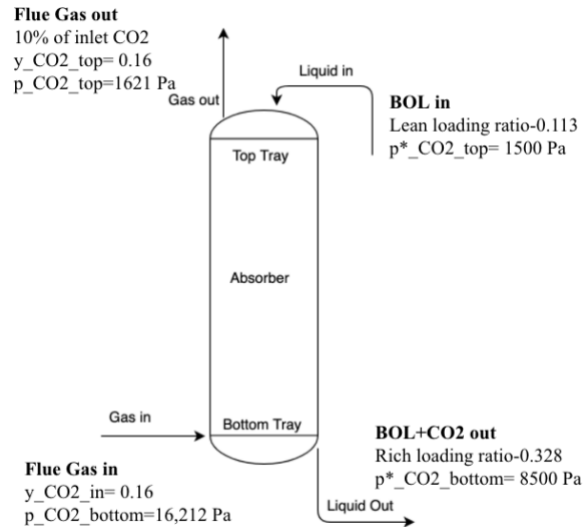


Figure 10.2. Visual of the absorption column. The column will take in the incoming flue gas at the bottom of the column and the EEMPA at the top. Leaving the top of the column will be the treated gas stream and leaving the bottom will be the bound BOL+CO₂ system. The column will be operated at 30°C and 1 atm.

The absorber is fed with an excess amount of EEMPA to maximize absorption. The BOL flow rate is adjusted to achieve the desired load of 0.328 moles of CO₂ per mole of BOL.

The column was sized with a mass-transfer approach since absorption is driven by the log-mean partial pressure difference of CO₂ in the EEMPA and CO₂ in the flue gas. Absorption is propelled by concentration differences of CO₂ in the EEMPA and CO₂ in the flue gas and this rate is dependent on the liquid film mass transfer coefficient of CO₂ in the EEMPA- CO₂ system. The original aspect ratio for the column was assumed to be 1:1, giving a size of 4.9 meters diameter and 4.9 meters height. However, in order to maintain the optimal temperature, interstage coolers are required and the height of the column needed to be increased. In order to account for the excess height, an aspect ratio of 5:1 was used, giving a diameter of 4 meters and a height of 20 meters.

The column is packed with Sulzer Mellapak 250Y Structured Packing (see Appendix B). This type of packing was chosen since it is most effective for columns of diameters up to 15 meters

and has a low pressure drop of 0.3-1 mbar per theoretical stage. Additionally, this packing works well for absorption of CO₂ in organic liquids.

Using a McCabe Thiele diagram (see Appendix A), it was determined that the absorption column required 5 theoretical stages to achieve the desired loading. CO₂ absorption is an exothermic process, and with CO₂ being absorbed at each stage of the column there is an increase in temperature at each stage. Therefore, the installation of intercoolers is required at stages 3 and 4 of the column, where they experience maximum temperature rises of 12°C and 18°C, respectively. These intercoolers use cooling water as coolant to limit the temperature rise of the absorption process to a maximum of 5°C.

6.4 Reactor

The process involves a continuous flow reaction through a packed bed reactor with Cu/ZnO/Al₂O₃ catalyst. The catalyst takes the form of raschig-ring like pellets to improve surface area. Despite the loss of efficiency involved with packed bed reactors, they tend to be the easiest and most simple to work with, making it ideal for this type of process.

The reactor design is based on the assumptions that the overall reaction rate is limited by mass transfer. This assumes that the H₂ instantaneously reacts when it enters the liquid, leaving the liquid side H₂ concentration at zero. Correlations concluded by Öztürk, Schumpe, and Deckwer were used to calculate the size of the absorption column (see Appendix A).

The hydrogen required for the reactor section was either to be made on site or to be bought and pumped in from an external source. The decision on hydrogen sourcing relied heavily on the siting of the process and the quantity of hydrogen needed. To minimize the environmental impact of the process while requiring 1,243 lb/hr H₂, the most economic option was to source H₂ from a

pipeline. Due to extensive H₂ pipelines, the process location was chosen to be the Gulf Coast region.

10.4 BOL Refining

Unable to directly and accurately model EEMPA in ASPEN, the final stages of separation were simulated using 1-Dodecanol,-2,2-Dimethyl (1-DOD-01), seen below in Figure 10.3. It was chosen because it has a molar mass of 214 kg/kmol, which is very similar EEMPA's molar mass of 216 kg/kmol.

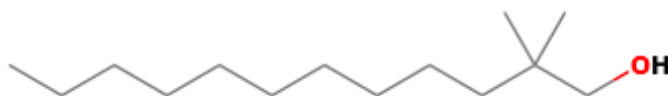


Figure 10.3 Molecular structure of 1-Dodecanol,-2,2-Dimethyl (1-DOD-01). With a similar structure and molar mass to EEMPA, 1-DOD-01 was selected to model the BOL in the simulation of the refining steps in Aspen.

Due to the non-volatile properties of our BOL, EEMPA, the BOL refining step was initially proposed to consist of a flash column followed by a distillation column. The BOL was to be separated from the water, methanol, and hydrogen in the flash column and recycled back to the absorber. The water, methanol, and hydrogen were to be separated in the distillation column, with the hydrogen leaving as a vapor distillate and recycled back to the reactor, and the methanol and water leaving in the liquid distillate and bottoms streams, respectively.

The process was initially planned to be completed with a flash column because of the equipment's ease in design and low costs. However, unable to achieve the desired separation within the flash column, the separation was attempted utilizing a decanter, yet was similarly unsuccessful. In order to understand the inability to separate EEMPA through flash distillation, we looked to the ASPEN produced ternary diagram seen in Figure 10.4 below. The ternary diagram

showed that liquid-liquid equilibrium was not achieved in the vessel, therefore disallowing a separation. Ultimately, with the recommendation of Professor Len Fabiano, we turned to the use of a distillation column, and with two distillation columns in series, the goal product of 99.6% pure methanol was obtained.

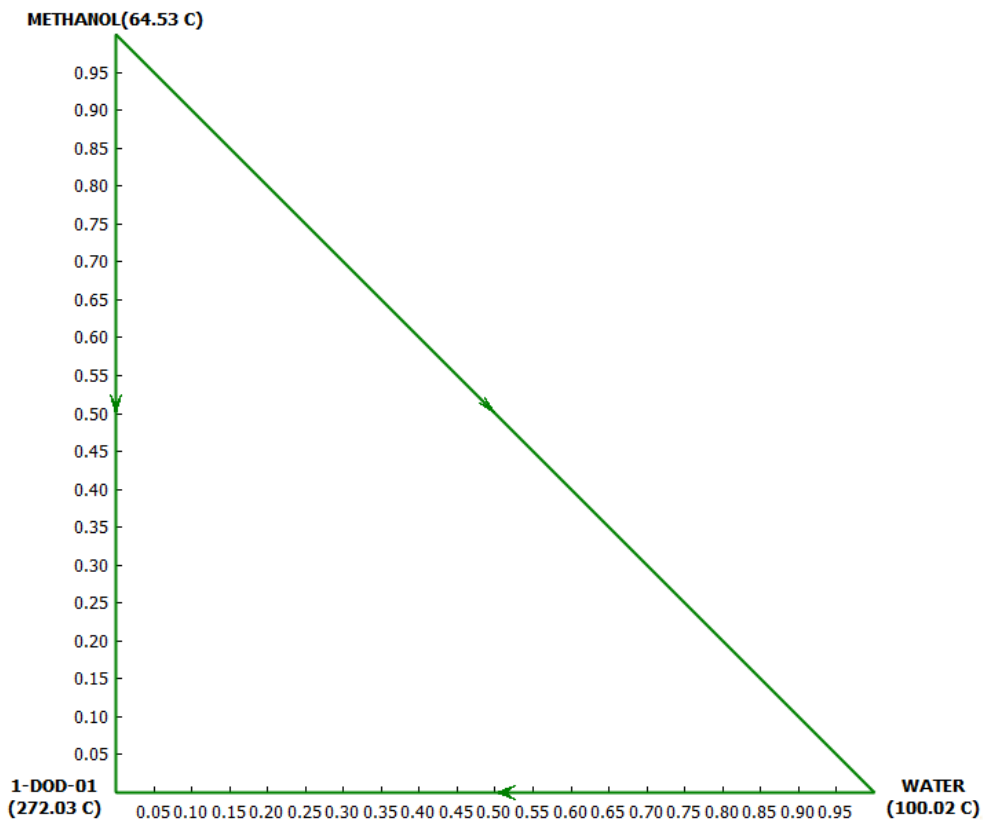


Figure 10.4 ASPEN produced ternary diagram for the mixture of methanol, water and dodecanol. Unable to achieve equilibrium, separation by flash vessel or decanter was unable to be realized.

With the utilization of two distillation columns to achieve the desired separation, a large compressor was required. This compressor needed to take the vapor overhead product from the first distillation column, leaving at 40 psia, and compress it to 25 bar to be recycled back into the reactor. Such a large and powerful compressor incurred a significant cost, so the idea of using a flash vessel was revisited. A new flash vessel was proposed to separate the hydrogen to be recycled from the water, methanol, and BOL. This added block was successful in maintaining the high

pressure of the hydrogen so that only a blower would be needed to recycle it back to the hydrogenation reactor. The rest of the mixture is then sent to two distillation columns, where EEMPA is separated out in the bottoms stream and recycled back to the absorber in the first distillation column, and in the second, methanol and water are separated to obtain methanol at a mass purity of 99.6%.

11. Assembly of Database

Table 11.1 Properties and Costs of Primary Chemicals

Chemical	Chemical Formula	Molar Mass (kg/kmol)	Boiling Point (°C)	Cost (\$USD/ton)
EEMPA	C ₁₁ N ₂ O ₂ H ₂₄	216.3	181	\$10,000
Hydrogen	H ₂	2.016	-253	\$1,250
Flue Gas	15.9% CO ₂ , 81.3% N ₂ , 2.8% O ₂	30.6	-	-

The cost of EEMPA presented above in Table 11.1 is an estimated target cost based on EEMPA's ability to be synthesized from relatively inexpensive raw materials with a single step process (Jaing et al., 2021).

The three graphs in Figure 11.1 below were used to plot equilibrium curves for CO₂ in the EEMPA system and to determine the mass transfer coefficients in order to size the absorption column. The graph on the left shows the relationship of equilibrium CO₂ pressure, P* with loading capacity, the middle shows its relationship to viscosity, and the graph on the right shows how loading changes with the liquid film mass transfer coefficient, kg'.

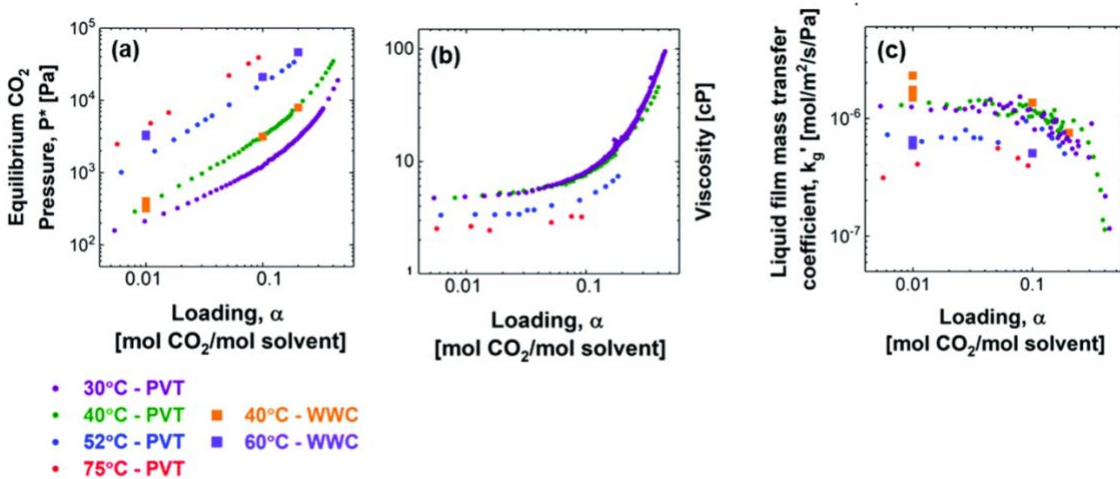


Figure 11.1 EEMPA properties with respect to loading capacity. The data for the graphs were obtained for both use with a pressure-volume-temperature column (PVT), as well as a wet wall column (WWC) at various temperatures. Our calculations were based off of the data collected for 30°C – PVT.

The first graph was used to determine the partial pressure of CO₂ in the BOL at the top and bottom of the column, which is used to calculate the log-mean CO₂ pressure difference. Similarly, the graph on the right is used to calculate the liquid film mass transfer coefficient at the entrance and exit of the column, which controls the rate of absorption.

The four graphs displayed in Figure 11.2 below were used to determine optimal operating conditions for the absorption column. From the two graphs on the top, relating pressure to CO₂ loading, it can be concluded that at higher pressure, the same levels of loading were achieved quicker. Additionally, higher pressure is required to achieve the same loading in a wet system when compared to a dry system. From the graph on the bottom left, we observed that viscosity increases as loading increases and viscosity also increases as water content increases. From the graph on the bottom right, we see that the mass transfer coefficient increases as the temperature decreases and the mass transfer coefficient increases as the water content increases. Therefore, operating conditions at a high pressure, low temperature, and low water content were deemed optimal for efficient absorption.

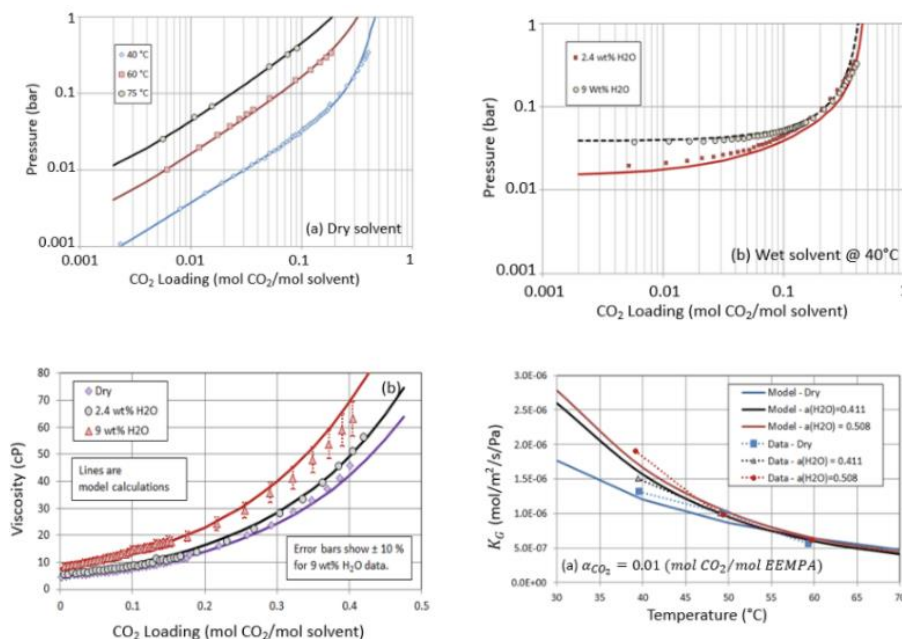


Figure 11.2 The four graphs above show EEMPA absorption VLE, viscosity, and mass transfer kinetic data. The data and conclusions obtained from analysis of these graphs informed the operating and design conditions of the absorption column used within our process.

12. Block Flow Diagram

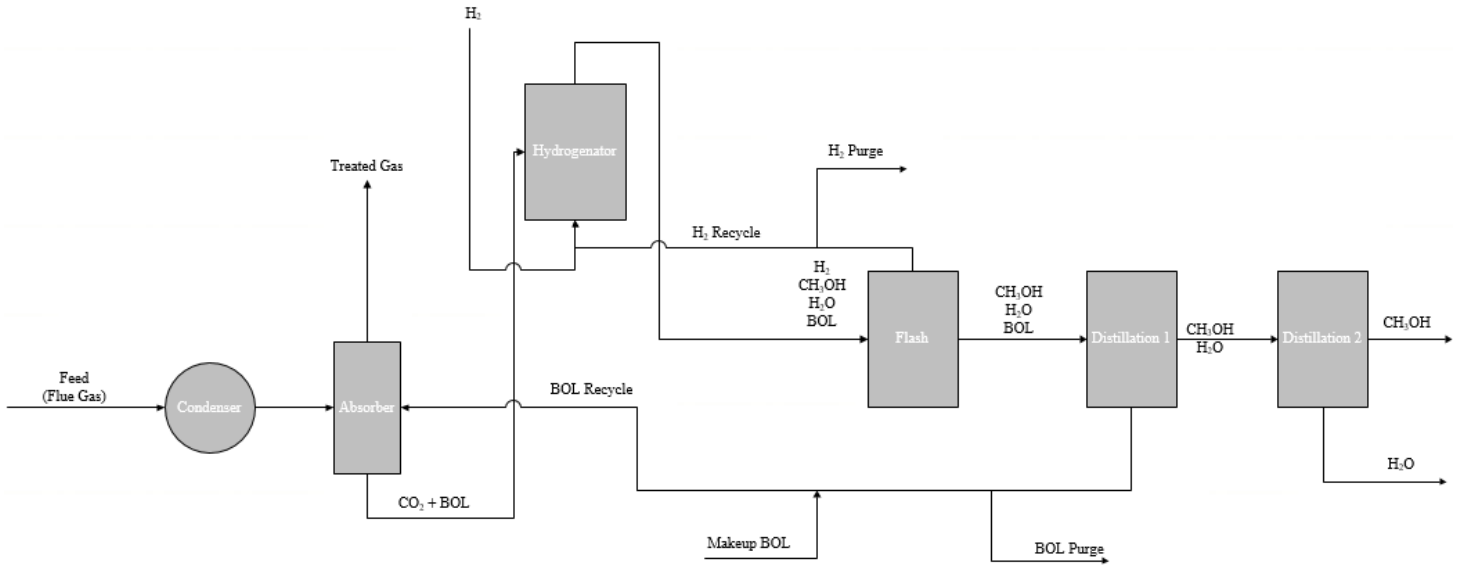


Figure 12.1 Block flow diagram for capture and conversion of CO₂ to methanol with EEMPA

13. Process Flow Diagram

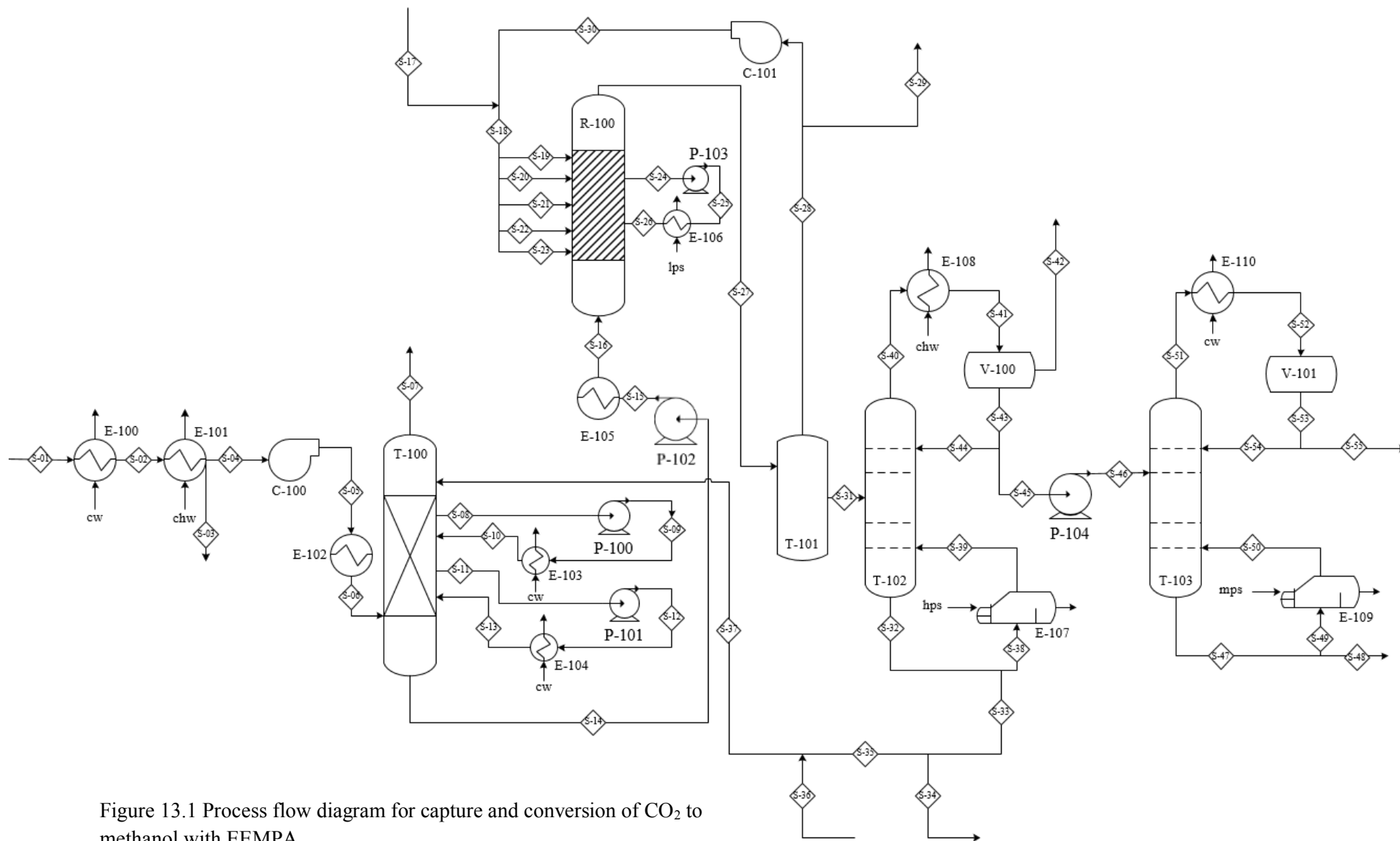


Figure 13.1 Process flow diagram for capture and conversion of CO₂ to methanol with EEMPA

13.1 Equipment Identifiers and Descriptions

E-100 Cooling water condenser	E-106 Heater
E-101 Chilled water condenser	T-101 Flash column
C-100 Blower	C-101 Blower
E-102 Heat exchanger	T-102 Distillation column
T-100 Absorption column	E-107 Kettle reboiler
P-100 Pump	E-108 Partial condenser
E-103 Intercooler	V-100 Reflux drum
P-101 Pump	P-104 Pump
E-104 Intercooler	T-103 Distillation tower
P-102 Pump	E-109 Kettle reboiler
E-105 Heat exchanger	E-110 Total condenser
R-100 Hydrogenation reactor column	V-101 Reflux drum
P-103 Pump	

14. Material Balances

Table 14.1 Stream Compositions and Conditions

Stream ID	S-01	S-02	S-03	S-04	S-05	S-06	S-07	S-08	S-09
Temperature (°C)	57	33	16	16	16	30	35	47	47
Pressure (bar)	1.10316	1.10316	1.10316	1.10316	1.01325	1.01325	1.01325	1.01325	1.01325
Total Mass Flow Rate (lb/hr)	53,763	53,763	9,141	44,623	44,623	44,623	35,458	254,178	254,178
Component Flow Rate (lb/hr)									
<i>CH₃OH</i>	-	-	-	-	-	-	-	-	-
<i>CO₂</i>	10,183	10,183	-	10,183	10,183	10183	1,018	2,306	2,306
<i>N₂ + Ar</i>	33,135	33,135	-	33,135	33,135	33135	33,135	33,135	33,135
<i>H₂O</i>	9,141	9,141	9,141	-	-	-	-	-	-
<i>NO_x</i>	-	-	-	-	-	-	-	-	-
<i>SO_x</i>	-	-	-	-	-	-	-	-	-
<i>O₂</i>	1,304	1,304	-	1,304	1,304	1304	1,304	1,304	1,304
<i>H₂</i>	-	-	-	-	-	-	-	-	-
<i>EEMPA</i>	-	-	-	-	-	-	-	170,829	170,829
<i>EEMPA+CO₂</i>	-	-	-	-	-	-	-	46,604	46,604

Stream ID	S-10	S-11	S-12	S-13	S-14	S-15	S-16	S-17	S-18
Temperature (°C)	35	53	53	35	35	35	120	120	120
Pressure (bar)	1.01325	1.01325	1.01325	1.01325	1.01325	25	25	25	25
Total Mass Flow Rate (lb/hr)	254,178	254,178	254,178	254,178	218,720	218,720	218,720	1,243	1,803.8
Component Flow Rate (lb/hr)									
<i>CH₃OH</i>	-	-	-	-	-	-	-	-	237.6
<i>CO₂</i>	2,306	5,316	5,316	5,316	-	-	-	-	-
<i>N₂ + Ar</i>	33,135	33,135	33,135	33,135	-	-	-	-	-
<i>H₂O</i>	-	-	-	-	-	-	-	-	43.2
<i>NO_x</i>	-	-	-	-	-	-	-	-	-
<i>SO_x</i>	-	-	-	-	-	-	-	-	-
<i>O₂</i>	1,304	1,304	1,304	1,304	-	-	-	-	-
<i>H₂</i>	-	-	-	-	-	-	-	1,243	1520.2
<i>EEMPA</i>	170,829	185,627	185,627	185,627	164,501	164,501	164,501	-	2.8
<i>EEMPA+CO₂</i>	46,604	28,796	28,796	28,796	54,219	54,219	54,219	-	-

Stream ID	S-19	S-20	S-21	S-22	S-23	S-24	S-25	S-26	S-27
Temperature (°C)	120	120	120	120	120	133	133	120	120
Pressure (bar)	25	25	25	25	25	24.5	25	25	25.0
Total Mass Flow Rate (lb/hr)	360.8	360.8	360.8	360.8	360.8	220,489.8	220,489.8	220,489.8	220,489.8
Component Flow Rate (lb/hr)									
<i>CH₃OH</i>	47.5	47.5	47.5	47.5	47.5	3,451.5	3,451.5	3,451.5	6,665.5
<i>CO₂</i>	-	-	-	-	-	-	-	-	-
<i>N₂ + Ar</i>	-	-	-	-	-	-	-	-	-
<i>H₂O</i>	8.6	8.6	8.6	8.6	8.6	1,816.5	1,816.5	1,816.5	3,624.3
<i>NO_x</i>	-	-	-	-	-	-	-	-	-
<i>SO_x</i>	-	-	-	-	-	-	-	-	-
<i>O₂</i>	-	-	-	-	-	-	-	-	-
<i>H₂</i>	304	304	304	304	304	917.6	917.6	917.6	315
<i>EEMPA</i>	0.6	0.6	0.6	0.6	0.6	186,228	186,228	186,228	207,952
<i>EEMPA+CO₂</i>	-	-	-	-	-	28,076.1	28,076.1	28,076.1	1,932.7

Stream ID	S-28	S-29	S-30	S-31	S-32	S-33	S-34	S-35	S-36
Temperature (°C)	120	120	120	120	139	139	139	139	139
Pressure (bar)	23.7	23.7	25.0	23.7	0.0887	0.0887	0.0887	0.0887	0.0887
Total Mass Flow Rate (lb/hr)	623	62.3	560.8	218,065	327,078	207,953	37.4	207,916	37.4
Component Flow Rate (lb/hr)									
<i>CH₃OH</i>	264	26.4	237.6	6,401	0.002	0	0	0	-
<i>CO₂</i>	-	-	-	-	-	-	-	-	-
<i>N₂ + Ar</i>	-	-	-	-	-	-	-	-	-
<i>H₂O</i>	48.0	4.80	43.2	3,702	8.47	4.24	0	4.24	-
<i>NO_x</i>	-	-	-	-	-	-	-	-	-
<i>SO_x</i>	-	-	-	-	-	-	-	-	-
<i>O₂</i>	-	-	-	-	-	-	-	-	-
<i>H₂</i>	308	30.8	277.2	4.00	0	0	0	0	-
<i>EEMPA</i>	3.12	0.312	2.8	207,949	327,070	207,949	37.4	207,912	37.4
<i>EEMPA+CO₂</i>	-	-	-	-	-	-	-	-	-

Stream ID	S-37	S-38	S-39	S-40	S-41	S-42	S-43	S-44	S-45
Temperature (°C)	139	139	189	29.6	10.2	10.2	10.2	10.2	10.2
Pressure (bar)	0.0887	0.0887	0.0887	0.0667	0.0667	0.0667	0.0667	0.0667	0.0667
Total Mass Flow Rate (lb/hr)	207,953	163,539	163,539	40,735	40,735	183	40,552	30,257	10,295
Component Flow Rate (lb/hr)									
<i>CH₃OH</i>	0	0	0	25,670	25,670	163	25,507	19,031	6,476
<i>CO₂</i>	-	-	-	-	-	-	-	-	-
<i>N₂ + Ar</i>	-	-	-	-	-	-	-	-	-
<i>H₂O</i>	4.24	4.24	4.24	15,062	15,062	16.8	15,045	11,226	3,819
<i>NO_x</i>	-	-	-	-	-	-	-	-	-
<i>SO_x</i>	-	-	-	-	-	-	-	-	-
<i>O₂</i>	-	-	-	-	-	-	-	-	-
<i>H₂</i>	0	0	0	3.49	3.49	3.47	0.005	0.004	0.001
<i>EEMPA</i>	207,949	163,535	163,535	0	0	0	0	0	0
<i>EEMPA+CO₂</i>	-	-	-	-	-	-	-	-	-

Stream ID	S-46	S-47	S-48	S-49	S-50	S-51	S-52	S-53	S-54	S-55
Temperature (°C)	11.0	128	128	128	133	95.2	94.9	94.9	94.9	94.9
Pressure (bar)	5.07	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00	3.00
Total Mass Flow Rate (lb/hr)	10,149	18,574	3,787	14,861	14,861	26,561	26,561	26,561	20,273	6,362
Component Flow Rate (lb/hr)										
<i>CH₃OH</i>	6,384	149	30.3	119	119	26,455	26,455	26,455	20,192	6,337
<i>CO₂</i>	-	-	-	-	-	-	-	-	-	-
<i>N₂ + Ar</i>	-	-	-	-	-	-	-	-	-	-
<i>H₂O</i>	3,765	18,425	3,757	14,742	14,742	106	106	106	81.1	25.4
<i>NO_x</i>	-	-	-	-	-	-	-	-	-	-
<i>SO_x</i>	-	-	-	-	-	-	-	-	-	-
<i>O₂</i>	-	-	-	-	-	-	-	-	-	-
<i>H₂</i>	0.001	0	0	0	0	0	0	0	0	0
<i>EEMPA</i>	0	0	0	0	0	0	0	0	0	0
<i>EEMPA+CO₂</i>	-	-	-	-	-	-	-	-	-	-

15. Process Descriptions

15.1 Flue Gas Feed

The flue gas providing CO₂ to our process is to be sourced from a coal power plant that has been treated by desulfurization (FGD). The option to source the flue gas from natural gas power plants was considered, as they have lower levels of nitrogen oxidizes and sulfur oxidizes without requiring any FGD pretreatment. Ultimately, due to the higher concentration of CO₂ in flue gas from coal fired power plants, and the increasing commonality of FGD treated flue gas, coal power plants were chosen. The temperature and pressure of the flue gas after FDG treatment will be 57°C and 15 psia respectively, with a composition of 15.9 mol% CO₂, 81.3 mol% N₂, 3.3 mol% O₂. Upon entering the process, the flue gas is chilled using cooling water from 57°C to 33°C and then to 16°C using chilled water. The purpose of this cooling process is to get a steady state of 1.6 wt.% of water in EEMPA as suggested by PNNL. The suggestion to reduce the amount of incoming water is based in data that has shown less water to result in lower capture costs. With less water, the system has a lower viscosity and thus requires a lower pressure to achieve the same loading (Jaing et al., 2021). The incoming flow of flue gas and all proceeding mass balances were based on the project goal to capture 100 tons of CO₂ per day.

15.2 CO₂ Absorption to BOL

The absorption column has been determined to require a diameter of 4 meters and a height of 20 meters in order to successfully absorb 90% of the incoming CO₂ onto the BOL within the absorption column. The design parameters were based upon an incoming lean loading ratio of

0.0113 mol CO₂/mol solvent and an outgoing rich loading ratio of 0.328 mol CO₂/mol solvent. Other important design parameters included the log mean difference in pressure between the top and the bottom of the column, the effective interfacial area of surface packing, and the liquid film mass transfer coefficient. These numbers were determined by sensitivity studies conducted by PNNL to optimize capture and regeneration pressure in relation to costs. The length to diameter ratio of 5:1 was chosen to minimize uneven liquid distribution concerns to maximize column efficiency as well as the goal to minimize the consumption of steel and other construction materials. The column pressure of 1 atm was deemed optimal based on sensitivity studies completed by PNNL that correlated column pressure with capture efficiency and price. Using data collected on the loading capacity's relationship with temperature, the operating temperature of the absorber was found to be most efficient at 30°C. The packing type is Mellapak Sulzer 250Y structured packing, which was chosen due to its wide use in industrial sized carbon capture columns (see pages in Appendix B). The absorption column contains five theoretical states, which was used to conduct a full energy analysis.

A sensitivity analysis on the energy and heat within the designed system showed that for every 5°C increase the mass transfer coefficient decreased by 0.25×10^{-6} . Utilizing this information and the fact that the total increase in temperature from stage five to stage one was 30°C, two interstage cooling water coolers are applied at stages three and four. The temperature of stage three is reduced by 12°C and the temperature of stage four is reduced by 18°C. Each interstage cooler is paired with a pump to provide a driving force for recirculation into the column. The waste gas produced within the absorber is removed from the top of the column.

15.3 Hydrogenation of Bound CO₂ to Methanol

The hydrogenation of CO₂ bound to EEMPA produces methanol and takes place in a packed bed reactor operating at 25 bar and 125°C, via the reaction shown in Equation 2 below. The operating pressure and temperature were chosen based on the maximization of conversion and the minimization of costs.



The goal was to design a continuous flow packed bed reactor using a Cu/ZnO/Al₂O₃ catalyst and to model it as an absorber. In order to model the reactor as an absorber, the overall reaction rate was assumed to be controlled by mass transfer so that once the hydrogen was in the liquid phase it was assumed to react instantaneously, leading to a concentration of zero H₂ on the liquid side. From Equation 3 below, the reaction vessel was found to be 1.3 meters in height and 0.6 meters in diameter:

$$reaction\ rate = k_{La} \times V_{reactor} \times C_{H_2} \quad (3)$$

where k_{La} is the mass transfer coefficient, $V_{reactor}$ is the volume of the reactor without catalyst, and C_{H_2} is the concentration of H₂ gas. The gas holdup and mass transfer coefficients were estimated from correlations provided by Ozturk, Schumpe, and Deckwer in “Organic Liquids in a Bubble Column: Holdups and Mass Transfer Coefficients” (see Appendix A).

In order to minimize superficial velocities to the studied ranges present in the reference paper, the reactor is split up into five separate sections each with a diameter of 0.6 meters and a height of 0.26 meters. A higher length to diameter ratio is typically desired, however, with design of the current system the superficial velocity of hydrogen gas would increase and exceed the range set forth by Ozturk, Schumpe, and Deckwer. The percentage of catalyst in the bed was set to be 60%.

In order to shift reaction equilibrium and increase conversion, H₂ is fed to the reactor in 25% excess based on the 3:1 stoichiometric ratio of H₂ to the EEMPA-CO₂ complex. The H₂ is fed through the sides of the reactor and the CO₂ bound EEMPA is pumped into the bottom of the reactor after leaving the bottom of the absorption column.

One of the main selling points of using EEMPA with our system is that the exothermicity of methanol production (-49.5 kJ/mol) can be paired with endothermicity of the sorbent regeneration (75 kJ/mol). In order to maintain an isothermal reaction, there is one interstage heater paired with a pump used to heat the reactor fluid by 14°C; without any extra heat, the total temperature rise would be 13°C.

15.4 BOL Refining and Methanol Separation

In order to obtain the desired purity of our methanol product, the various components exiting in the outlet stream from the reactor need to be separated. The main objective of the process is to achieve a methanol product with 99.6% purity, along with the additional goal of wasting minimal amounts of EEMPA and H₂. Under the guidance of Professor Len Fabiano, the separation process was entirely modeled in Aspen, with results reported in Appendix A. EEMPA was modeled using 1-Dodecanol,-2,2-Dimethyl (1-DOD-01) because EEMPA could not be accurately input into the Aspen simulation. 1-DOD-01 was chosen for its similar structure and molar mass, as previously seen in Figure 10.3.

The first step of the separation process is the removal of H₂ from the fluid through a flash vessel, specified in section 18. A one-stage flash is used to maintain a high pressure in the stream, allowing for a small amount of work to get the vapor overhead stream back to the 25 bar operating

pressure of the hydrogenation reactor. The flash vapor stream contains 49.5% H₂ and is recycled back into the hydrogenation reactor to contribute to further reactions.

A three-stage flash was considered in the initial stages of process design with the goal of separating the H₂ and the EEMPA within the same vessel in the vapor overhead and bottoms streams respectively. This was an attractive option because it would have reduced the process equipment by requiring simply a flash column followed by a distillation column. The process was assumed to have a high potential for success due to the large mass differences between the H₂, EEMPA, and methanol and water. With further analysis, this was not deemed to be a feasible option as there was no successful separation between EEMPA and the methanol and water mixture. This separation was unsuccessful because liquid-liquid equilibrium could not be achieved between the EEMPA and the methanol and water mixture. Attempting to drive the formation of two liquid phases, the pressure in the column was significantly reduced, however, even at pressures as low as 1 bar, EEMPA could not be separated out. Analyzing the vapor-liquid equilibrium and ternary diagrams produced by Aspen, shown in Figure 10.4, we saw that a liquid-liquid equilibrium separation of this kind was not possible.

Additionally, a decanter was considered to complete the separation of EEMPA from methanol and water. This attempt was likewise unsuccessful, and the separation was not achieved.

With the first step of a flash column needed to separate out the hydrogen for recycling, the next step was to separate out the EEMPA. The EEMPA is separated for recycle through a distillation column specified in section 18.

Once EEMPA is removed from the stream, a nearly pure mixture of methanol and water remains. A second distillation column is needed to separate these two components and is specified in section 18. To create a driving force for the fluid to move from the first distillation column and

into the second, a pump, specified in section 18, is required. This pump takes advantage of using pressure as a driving force and makes up for any pressure that may be lost between the two distillation columns. The minimum change in pressure to account for the loss of pressure and to provide a useful driving force is estimated to be 15 psi by recommendation of Professor Len Fabiano. In order to move the quantity of fluid at a respectable pace without incurring large, unnecessary costs, a pump to increase the pressure by 5 bar is incorporated into the process.

Once the fluid passes through the pump, it flows into the final distillation column where water and methanol are separated. The specifications of this distillation column are recorded on page of section 18. A design spec is input into Aspen to ensure production of methanol at the desired purity of 99.6 mass%.

15.5 Hydrogen Recycle

Due to the excess amount of hydrogen fed to the reactor in order to shift equilibrium and increase conversion, unreacted H₂ remains within the stream to be recycled back to the hydrogenator after the flash vessel. The hydrogen separated in the overhead stream of the flash vessel exits at 24 bar and is passed through a blower to increase the pressure to 25 bar. Once the H₂ recycle stream matches the pressure of the H₂ feed, the recycle stream is joined with the incoming hydrogen stream coming from the hydrogen pipeline. The flash vessel was designed to operate at high pressures so that a compressor would not be needed for the H₂ recycle. Due to impurities in the hydrogen source 10% of the recycle stream, 62.3lb/hr, is purged to avoid the buildup of these impurities.

15.6 BOL Recycle

Due to the high cost of our BOL, conserving and recycling as much EEMPA as possible is a priority. EEMPA is separated out from the stream in the bottoms of the first distillation column is then sent back to be recycled into the absorber. According to PNNL, there is 3% solvent loss every 5 weeks (personal communication), and due to this and the degradation of EEMPA over time, the recycle stream includes a purge and makeup stream. The purge stream will be collected and sent back to the EEMPA supplier at a rate of 37.4 lb/hr. In order to maintain an uninterrupted process flow, the makeup stream will similarly be 37.4 lb/hr.

16. Energy Balance and Utility Requirements

Table 16.1 Utility Requirements and Costs

Equipment Type	Unit No.	Power (kWh)	Price (\$/kWh)	Annual Consumption (kWh)	Annual Price (\$/yr)
Condenser	E-100	-	-	-	\$1,529
Condenser	E-101	-	-	-	\$41,003
Blower	C-100	3.3	0.07	26136	\$1,830
Heater	E-102	-	-	-	\$1,730
Absorber	T-100	-	-	-	-
Pump	P-100	2.1	0.07	16632	\$1,164
Intercooler	E-103	-	-	-	\$9,121
Pump	P-101	2.1	0.07	16632	\$1,164
Intercooler	E-104	-	-	-	\$14,361
Pump	P-102	96	0.07	760320	\$53,222
Heater	E-105	-	-	-	\$20,473
Reactor	R-100	-	-	-	-
Pump	P-103	2.1	0.07	16632	\$1,164
Heater	E-106	-	-	-	\$21,131
Blower	C-101	2.6	0.07	20592	\$1,441
Flash Column	T-101	-	-	-	-
Distillation Column	T-102	-	-	-	-
Partial Condenser	E-108	-	-	-	\$2,583,019
Reboiler	E-107	-	-	-	\$265,498
Reflux Drum	V-100	-	-	-	-
Pump	P-104	2.28	0.07	18058	\$1,264

Equipment Type	Unit No.	Power (kWh)	Price (\$/kWh)	Annual Consumption (kWh)	Annual Price (\$/yr)
Distillation Column	T-103	-	-	-	-
Total Condenser	E-110	-	-	-	\$24,469
Reboiler	E-109	-	-	-	\$88,898
Reflux Drum	V-101	-	-	-	-

17. Equipment List and Unit Descriptions

17.1 Condensers

E-100

E-100 is the first condenser to take in the flue gas feed. Using cooling water, it is a shell and tube heat exchanger that reduces the temperature of the flue gas from 57°C to 33°C, with the purpose of removing water from the flue gas. Data collected by Jaing, et al. has suggested that reducing the amount of water entering the process will result in lower capture costs. With less water, the system has a lower viscosity and thus requires a lower pressure to achieve the same level of loading (Jaing et al., 2021). The surface area of this heat exchanger is 4,937 ft² and the log mean temperature difference is 6°C. The purchase cost of the condenser is \$258,093.

E-101

E-101 is the second condenser to take in the flue gas feed. Using chilled water, it is a shell and tube heat exchanger that reduces the temperature of the flue gas from 33°C to 16°C, with the goal of further condensing and removing as much water from the flue gas as possible. Data collected by Jaing, et al. has suggested that reducing the amount of water entering the process will result in lower capture costs. With less water, the system has a lower viscosity and thus requires a lower pressure to achieve the same level of loading (Jaing et al., 2021). The area is 3,314 ft² and the log mean temperature difference is 6°C. The purchase cost of the condenser is \$201,189..

17.2 Blowers

C-100

C-100 is a blower used to transport the cooled flue gas into the absorption column using pressure as a driving force. It is a centrifugal blower and consumes approximately 3 kW. It is constructed out of cast iron. The incoming flue gas is at 16°C and has a flow rate of 44,623 lb/hr and at a pressure of 15 psia. The purchase cost of the blower is \$8,224.

17.3 Heat Exchangers

E-102

E-102 is a shell and tube heat exchanger used to heat the flue gas to match the absorber operating temperature. The surface area required is 5 ft² and the log mean temperature difference is 88°C. The heat exchanger is made from carbon steel and has a tube length of 12 ft. The purchase cost of the heat exchanger is \$77,011.

E-103

E-103 is a shell and tube heat exchanger used to cool the absorber so that the mass transfer coefficients for the EEMPA-CO₂ system do not drastically decrease. It cools from stage 4, 17°C and the surface area required is 2,968 ft². The log mean temperature difference is 12. It is made from carbon steel and has a tube length of 12 feet. The purchase cost of the heat exchanger is \$188,745.

E-104

E-104 is an interstage shell and tube heat exchanger used to cool the absorber so that the mass transfer coefficients for the EEMPA-CO₂ system do not drastically decrease. It cools the absorber at stage 3 by 11°C with a required surface area of 3,249 ft². The log mean temperature

difference is 7°C and it is made from carbon steel with a tube length of 12 feet. The purchase cost of the heat exchanger is \$198,862.

E-105

E-105 is a shell and tube heat exchanger used to heat the EEMPA-CO₂ system to match the reactor operating temperature. The surface area required is 2,478 ft² and the log mean temperature difference is 12°C. It is made from carbon steel and has a tube length of 12 feet. The purchase cost of the heat exchanger is \$170,825.

E-106

E-106 is a shell and tube heat exchanger used to heat the reactor to maintain isothermal conditions to ensure that the reaction kinetics are not significantly affected as the reaction continues. From the second section, it heats the reactor by 13°C and requires a surface area of 1,181 ft². The log mean temperature difference is 26°C and it is made from carbon steel and has a tube length of 12 feet. The purchase cost of the heat exchanger is \$128,782.

E-107

E-107 is a kettle reboiler associated with the first distillation column. It is a shell and tube heat exchanger used to provide the bottom tray of the column with a vapor stream. The temperature of the reboiler is 198°C and the reboiler duty is 41 million BTUs/hr. The surface area is 1,462 ft², and it is constructed out of carbon steel. The purchase cost of the reboiler is \$131,968.

E-108

E-108 is a partial condenser associated with the first distillation column. It is a shell and tube heat exchanger used to condense some of the vapor leaving the top of the column to provide for a liquid reflux stream to flow back into the column and a liquid distillate to leave the column. The temperature of the condenser is 33°C and the pressure is 40 psia with a heat duty of 30 million BTUs/hr. The required surface area of the heat exchanger is 11,634 ft² and it is constructed out of carbon steel. The purchase cost of the partial condenser is \$485,836.

E-109

E-109 is a kettle reboiler associated with the second distillation column. It is a shell and tube heat exchanger used to provide the bottom tray of the column with a vapor stream. The temperature of the reboiler is 125°C and the reboiler duty is 13 million BTUs/hr. The required surface area is 436 ft², and it is constructed out of carbon steel. The purchase cost of the reboiler is \$88,243.

E-110

E-110 is a total condenser associated with the second distillation column. It is a shell and tube heat exchanger used to condense the vapor leaving the top of the column to provide for a liquid reflux stream to flow back into the column and a liquid distillate to leave the column. The operating temperature of the condenser is 21°C and the pressure is 44 psia. The condenser duty is 11 million BTUs/hr with a required surface area of 582 ft². It is constructed out of carbon steel and the purchase cost of the total condenser is \$94,843.

17.3 Absorption Tower

T-100

T-100 is an absorption tower used to absorb CO₂ onto the binding organic liquid EEMPA. The tower is designed to be 4 meters in diameter and 20 meters in height and will be operated at a pressure of 1 atm and a temperature 30°C. Since the vessel is made out of carbon steel, the maximum allowable stress is 13,750 psig. The absorption tower will be packed with Sulzer MellaPak 250 Y structured packing, with cost estimates obtained from the vendor website (see Appendix B). The flue gas will enter the absorber at a mass flow rate of 44,623 lb/hr along with 209,555 lb/hr of EEMPA. In order to prevent a decrease in the mass transfer coefficient of the EEMPA-CO₂ system, the reactor has two interstage coolers incorporated at stages 3 and 4 to cool the tower 12 and 18 degrees each. The purchase cost of the absorption tower is \$1,158,622.

17.4 Pumps

P-100

P-100 is an external gear pump that pumps the fluid from the absorption tower into the interstage cooler (E-103) at stage 4. The interstage cooler is used to prevent a decrease in the mass transfer coefficient, and the pump provides a pressure driving force to ensure the fluid flows easily through the heat exchanger. The pump will handle a flowrate of 513 gal/min. The pump will be made of cast iron with a purchase cost of \$40,340.

P-101

P-101 is an external gear pump that pumps the fluid from the absorption tower into the interstage cooler (E-104) at stage 3. The interstage cooler is used to prevent a decrease in the mass transfer coefficient, and the pump provides a pressure driving force to ensure the fluid flows easily through the heat exchanger. The pump needs to handle a flowrate of 510 gal/min. The pump will be made of cast iron with a purchase cost of \$40,198.

P-102

P-102 is a centrifugal pump that pumps from the fluid leaving the bottom of the absorber into the reactor. The pump will handle a flowrate of 445 gal/min and the pump head is calculated to be 991 feet. The pump will be made of cast iron with a purchase cost of \$31,079.

P-103

P-103 is an external gear pump that pumps the fluid from the reactor vessel into the interstage cooler (E-106) after the second section. The interstage cooler is used to maintain isothermal reaction conditions and allow for constant reaction kinetics, while the pump provides a pressure driving force to ensure the fluid flows easily through the heat exchanger. The pump will handle a flowrate of 4,969 gal/min. The pump will be made of cast iron with a purchase cost of \$250,382.

P-104

P-104 is a centrifugal pump that pumps the liquid distillate leaving from the top of the first distillation column into the second distillation column. The pump will handle a flowrate of 23 gal/min and the pump head is calculated to be 195 ft. The pump will be made of cast iron with a purchase cost of \$15,979.

17.5 Hydrogenation Reactor

R-100

R-100 is the hydrogenation reactor vessel and is used to convert the EEMPA-CO₂ bound system into methanol. Hydrogen is fed to the reactor in a 25% excess based on the three to one stoichiometric ratio of hydrogen to the produced methanol. The reactor is 1.3 meters in height and 0.6 meters in diameter and split into five separate sections in order to maintain low hydrogen gas

superficial velocities of 0.08 ms^{-1} . The reactor operates at 25 bar and 125°C in order to shift the reaction towards the production methanol. The flow rate into the reactor is 218,720 lb/hr, which consists of EEMPA and EEMPA bound to carbon dioxide. Hydrogen gas is supplied to the reactor using a pipeline at a flow rate of 1,243 lb/hr. This merges with the recycle stream (consisting of hydrogen, water, methanol and EEMPA) having a flow rate of 560.8 lb/hr. With the vessel being made out of carbon steel, the maximum allowable stress is 13,750 psig. There is one interstage heater incorporated into the reactor to maintain isothermal reaction conditions and to help regenerate EEMPA. The purchase cost of the reactor is \$90,266.

17.6 Flash Vessel

T-101

T-101 is the flash vessel used to separate out hydrogen from water, EEMPA, and methanol. It is the first separation unit after the reactor and operates with zero heat duty. The height of the vessel is 19.28 ft, and the diameter of the vessel is 4.79 ft. The vessel will operate at a temperature and pressure of 120°C and 23.7 bar respectively. The flash vapor overhead stream contains 49.5% H_2 and is recycled back into the hydrogenation reactor. The purchase cost of the flash vessel is \$307,899.

17.7 Distillation Towers - BOL Separation

T-102

The first of the two distillation columns is used to separate EEMPA from water and methanol. The column is 4 meters in diameter, 20 meters in height, and the operating pressure is 1 psig. The distillation tower will be constructed out of carbon steel and sieve trays will be used. There are 22 stages and the incoming feed will be fed to stage 16. The incoming feed is at 120°C and 24 bar and the total flow rate is 174,605 lb/hr. The purchase cost of the tower is \$1,335,925.

T-103

The second of the two distillation columns is used to separate methanol and water. The column is 1 meter in diameter, 17 meters in height and the operating pressure is 43 psig. The distillation tower will be constructed out of carbon steel and sieve trays will be used. There are 30 stages and the feed stage is stage 16. The incoming feed is at 11°C and 5 bar and the total flow rate is 10,149 lb/hr. The purchase cost of the tower is \$1,335,925.

18. Specification Sheets

Condenser 1			
Identification	Item	<i>Condenser</i>	Date. 3/30
	Item No.	<i>E-100</i>	By. AK
	No. Required	1	
Function	Cool down flue gas		
Operation	Continuous		
Materials Handled			
Stream ID		S-01	S-02
	Quantity (lb/hr)	53,763	53,763
	Mass Composition:		
	<i>CO₂</i>	10,183	10,183
	<i>N₂ + Ar</i>	33,135	33,135
	<i>H₂O</i>	9,141	9,141
	<i>NO_x</i>	-	-
	<i>SO_x</i>	-	-
	<i>O₂</i>	1,304	1,304
	<i>H₂</i>	-	-
	<i>EEMPA</i>	-	-
	<i>EEMPA+CO₂</i>	-	-
	<i>CH₃OH</i>	-	-
	Temperature (°C)	57	33
	Pressure (bar)	1.1	1.1
Design Data			
	Cross Sectional Area	4,937 ft ²	
	Overall Heat Transfer Coefficient	20 BTU/ °F-ft ² -hr	
Utility Requirements	16,113 lb/hr cooling water		
Comments	See Process Flow Diagram		

Condenser 2				
Identification	Item	<i>Condenser</i>	Date.	3/30
	Item No.	<i>E-102</i>	By.	AK
	No. Required	1		
Function	Cool down flue gas to remove water			
Operation	Continuous			
Materials Handled		S-02	S-03	S-04
Stream ID	Quantity (lb/hr)	53,763	9,141	44,623
	Mass Composition:			
	<i>CO₂</i>	10,183	-	10,183
	<i>N₂ + Ar</i>	33,135	-	33,135
	<i>H₂O</i>	9,141	-	-
	<i>NO_x</i>	-	-	-
	<i>SO_x</i>	-	-	-
	<i>O₂</i>	1,304	1,304	1,304
	<i>H₂</i>	-	-	-
	<i>EEMPA</i>	-	-	-
	<i>EEMPA+CO₂</i>	-	-	-
	<i>CH₃OH</i>	-	-	-
	Temperature (°C)	57	33	16
Design Data	Cross Sectional Area	3,313 ft ²		
	Overall Heat Transfer Coefficient	20 BTU/ °F-ft ² -hr		
Utility Requirements	7,609 lb/hr chilled water			
Comments	See Process Flow Diagram			

Blower			
Identification	Item	<i>Blower</i>	Date. 3/30
	Item No.	<i>C-100</i>	By. AK
	No. Required	1	
Function	Blow flue gas into heat exchanger for absorption column		
Operation	Continuous		
Materials Handled			
Stream ID		S-04	S-05
	Quantity (lb/hr)	44,623	44,623
	Mass Composition:		
	<i>CO₂</i>	10,183	10,183
	<i>N₂ + Ar</i>	33,135	33,135
	<i>H₂O</i>	-	-
	<i>NO_x</i>	-	-
	<i>SO_x</i>	-	-
	<i>O₂</i>	1,304	1,304
	<i>H₂</i>	-	-
	<i>EEMPA</i>	-	-
	Temperature (°C)	16	16
	Pressure (bar)	1.1	1.01
	Vapor Fraction	-	-
Design Data			
	Temperature	16 C	
	Pressure	1.1 bar	
Utility Requirements	Net Work Required: 3.3 kW		
Comments	See Process Flow Diagram		

Heat Exchanger			
Identification	Item	<i>Heat Exchanger</i>	Date. 3/30
	Item No.	<i>E-102</i>	By. YA
	No. Required	1	
Function	Heat flue gas going into absorption column		
Operation	Continuous		
Materials Handled			
Stream ID		S-05	S-06
	Quantity (lb/hr)	44,623	44,623
	Mass Composition:		
	<i>CO₂</i>	10,183	10,183
	<i>N₂ + Ar</i>	33,135	33,135
	<i>H₂O</i>	-	-
	<i>NO_x</i>	-	-
	<i>SO_x</i>	-	-
	<i>O₂</i>	1,304	1,304
	<i>H₂</i>	-	-
	<i>EEMPA</i>	-	-
	Temperature (°C)	16	30
	Pressure (bar)	1.01	1.01
	Vapor Fraction	-	-
Design Data			
	Cross Sectional Area	5 ft ²	
	Overall Heat Transfer Coefficient	200 BTU/ °F-ft ² -hr	
Utility Requirements	36.4 lb/hr low pressure steam		
Comments	See Process Flow Diagram		

Absorber				
Identification	Item	<i>Absorber Column</i>		Date. 3/30
	Item No.	T-100		By. YA
	No. Required	1		
Function	Absorb CO ₂ onto EEMPA			
Operation	Continuous			
Materials Handled Stream ID		S-06	S-07	S-14
	Quantity (lb/hr)	44,623	35,458	218,720
	Mass Composition:			
	<i>CO₂</i>	10,183	1,018	-
	<i>N₂ + Ar</i>	33,135	33,135	-
	<i>H₂O</i>	-	43.2	-
	<i>NO_x</i>	-	-	-
	<i>SO_x</i>	-	-	-
	<i>O₂</i>	1,304	1,304	-
	<i>H₂</i>	-	1520.2	-
	<i>EEMPA</i>	-	-	164,501
	<i>EEMPA+CO₂</i>	-	-	54,219
	<i>CH₃OH</i>	-	-	-
Temperature (°C)	30	30	35	
Pressure (bar)	1.01	1.01	1.01	
Design Data	Operating Temperature	30 °C		
	Operating Pressure	1.01 bar		
	Number of Stages	5		
	Reactor Height	20 m		
	Reactor Diameter	4 m		
	Packing Type	Sulzer Mellapak 250Y		
Utility Requirements	5,691,017 BTU/hr cooling required			
Comments	See Process Flow Diagram			

Pump			
Identification	Item	<i>Pump</i>	Date. 3/30
	Item No.	<i>P-100</i>	By. AK
	No. Required	1	
Function	Pump EEMPA-CO ₂ system to heat exchanger for cooling		
Operation	Continuous		
Materials Handled Stream ID	Quantity (lb/hr)	S-08 254,178	S-09 254,178
	Mass Composition:		
	<i>CO₂</i>	2,306	2,306
	<i>N₂ + Ar</i>	33,135	33,135
	<i>H₂O</i>	-	-
	<i>NO_x</i>	-	-
	<i>SO_x</i>	-	-
	<i>O₂</i>	1,304	1,304
	<i>H₂</i>	-	-
	<i>EEMPA</i>	170,829	170,829
	<i>EEMPA+CO₂</i>	46,604	46,604
	<i>CH₃OH</i>	-	-
	Temperature (°C)	47	35
Pressure (bar)	1.01	1.01	
Design Data	Temperature	47 C	
	Pressure	1.01 bar	
Utility Requirements	Net Work Required: 2.1kW		
Comments	See Process Flow Diagram		

Heat Exchanger			
Identification	Item	<i>Heat Exchanger</i>	Date. 3/30
	Item No.	<i>E-103</i>	By. YA
	No. Required	1	
Function	Cool down EEMPA-CO ₂ system		
Operation	Continuous		
Materials Handled Stream ID		S-09	S-10
	Quantity (lb/hr)	254,178	254,178
	Mass Composition:		
	<i>CO₂</i>	2,306	2,306
	<i>N₂ + Ar</i>	33,135	33,135
	<i>H₂O</i>	-	-
	<i>NO_x</i>	-	-
	<i>SO_x</i>	-	-
	<i>O₂</i>	1,304	1,304
	<i>H₂</i>	-	-
	<i>EEMPA</i>	170,829	170,829
	<i>EEMPA+CO₂</i>	46,604	46,604
	<i>CH₃OH</i>	-	-
Temperature (°C)	47	35	
Pressure (bar)	1.01	1.01	
Design Data	Cross Sectional Area	3,249 ft ²	
	Overall Heat Transfer Coefficient	100 BTU/ °F-ft ² -hr	
Utility Requirements	96,111 lb/hr cooling water		
Comments	See Process Flow Diagram		

Pump			
Identification	Item	<i>Pump</i>	Date. 3/30
	Item No.	<i>P-101</i>	By. AK
	No. Required	1	
Function	Pump EEMPA-CO ₂ system to next interstage cooler		
Operation	Continuous		
Materials Handled			
Stream ID		S-11	S-12
	Quantity (lb/hr)	254,178	254,178
	Mass Composition:		
	<i>CO₂</i>	5,316	5,316
	<i>N₂ + Ar</i>	33,135	33,135
	<i>H₂O</i>	-	-
	<i>NO_x</i>	-	-
	<i>SO_x</i>	-	-
	<i>O₂</i>	1,304	1,304
	<i>H₂</i>	-	-
	<i>EEMPA</i>	185,627	185,627
	<i>EEMPA+CO₂</i>	28,796	28,796
	<i>CH₃OH</i>	-	-
	Temperature (°C)	53	53
	Pressure (bar)	1.01	1.01
Design Data			
	Temperature	53 C	
	Pressure	1.01 bar	
Utility Requirements	Net Work Required: 2.1 kW		
Comments	See Process Flow Diagram		

Heat Exchanger			
Identification	Item	<i>Heat Exchanger</i>	Date. 3/30
	Item No.	<i>E-104</i>	By. YA
	No. Required	1	
Function	Cool down EEMPA-CO ₂ system		
Operation	Continuous		
Materials Handled		S-12	S-13
Stream ID	Quantity (lb/hr)	254,178	254,178
	Mass Composition:		
	<i>CO₂</i>	5,316	5,316
	<i>N₂ + Ar</i>	33,135	33,135
	<i>H₂O</i>	-	-
	<i>NO_x</i>	-	-
	<i>SO_x</i>	-	-
	<i>O₂</i>	1,304	1,304
	<i>H₂</i>	-	-
	<i>EEMPA</i>	185,627	185,627
	<i>EEMPA+CO₂</i>	28,796	28,796
	<i>CH₃OH</i>	-	-
	Temperature (°C)	35	35
	Pressure (bar)	1.01	1.01
Design Data	Cross Sectional Area	2,968 ft ²	
	Overall Heat Transfer Coefficient	100 BTU/ °F-ft ² -hr	
Utility Requirements	151,324 lb/hr cooling water		
Comments	See Process Flow Diagram		

Pump			
Identification	Item	<i>Pump</i>	Date. 3/30
	Item No.	<i>P-102</i>	By. AK
	No. Required	1	
Function	Pump EEMPA-CO ₂ towards heat exchanger then reactor		
Operation	Continuous		
Materials Handled		S-14	S-15
Stream ID	Quantity (lb/hr)	218,720	218,720
	Mass Composition:		
	<i>CO₂</i>	-	-
	<i>N₂ + Ar</i>	-	-
	<i>H₂O</i>	-	-
	<i>NO_x</i>	-	-
	<i>SO_x</i>	-	-
	<i>O₂</i>	-	-
	<i>H₂</i>	-	-
	<i>EEMPA</i>	164,501	164,501
	<i>EEMPA+CO₂</i>	54,219	54,219
	<i>CH₃OH</i>	-	-
	Temperature (°C)	35	35
	Pressure (bar)	1.01	25
Design Data	Temperature	35 C	
	Pressure	25 bar	
Utility Requirements	Net Work Required: 96 kW		
Comments	See Process Flow Diagram		

Heat Exchanger			
Identification	Item	<i>Heat Exchanger</i>	Date. 3/30
	Item No.	<i>E-105</i>	By. YA
	No. Required	1	
Function	Heat EEMPA-CO ₂ system to reactor temperature		
Operation	Continuous		
Materials Handled			
Stream ID		S-15	S-16
	Quantity (lb/hr)	218,720	218,720
	Mass Composition:		
	<i>CO₂</i>	-	-
	<i>N₂ + Ar</i>	-	-
	<i>H₂O</i>	-	-
	<i>NO_x</i>	-	-
	<i>SO_x</i>	-	-
	<i>O₂</i>	-	-
	<i>H₂</i>	-	-
	<i>EEMPA</i>	164,501	164,501
	<i>EEMPA+CO₂</i>	54,219	54,219
	<i>CH₃OH</i>	-	-
	Temperature (°C)	35	120
	Pressure (bar)	25	25
Design Data			
	Cross Sectional Area	2,478 ft ²	
	Overall Heat Transfer Coefficient	75 BTU/ °F-ft ² -hr	
Utility Requirements	431 lb/hr low pressure steam		
Comments	See Process Flow Diagram		

Reactor				
Identification	Item	<i>Reactor</i>	Date	3/30
	Item No.	R-100	By	YA
	No. Required	1		
Function	Hydrogenate CO ₂ into methanol			
Operation	Continuous			
Materials Handled Stream ID	Quantity (lb/hr)	S-16	S-18	S-27
		218,720	1,803.8	220,489.8
	Mass Composition:			
	<i>CO₂</i>	10,183	-	-
	<i>N₂ + Ar</i>	-	-	-
	<i>H₂O</i>	-	43.2	-
	<i>NO_x</i>	-	-	-
	<i>SO_x</i>	-	-	-
	<i>O₂</i>	-	-	-
	<i>H₂</i>	-	1520.2	315
	<i>EEMPA</i>	164,501	2.8	207,952.2
	<i>EEMPA+CO₂</i>	54,219	-	1932.7
	<i>CH₃OH</i>	-	237.6	6665.5
	Temperature (°C)	120	120	120
Pressure (bar)	25	25	25	
Design Data	Operating Temperature	120 °C		
	Operating Pressure	25 bar		
	Number of Stages	5		
	Reactor Height	0.6 m		
	Reactor Diameter	1.3 m		
	Catalyst Type	Cu/ZnO/Al ₂ O ₃		
Utility Requirements	2,296,087 BTU/hr heating required			
Comments	See Process Flow Diagram			

Pump			
Identification	Item	<i>Pump</i>	Date. 3/30
	Item No.	<i>P-103</i>	By. AK
	No. Required	1	
Function	Pump flue gas to interstage heater		
Operation	Continuous		
Materials Handled Stream ID	Quantity (lb/hr)	S-24	S-25
		220,489.8	220,489.8
	Mass Composition:		
	<i>CO₂</i>	-	-
	<i>N₂ + Ar</i>	-	-
	<i>H₂O</i>	1,874	1,874
	<i>NO_x</i>	-	-
	<i>SO_x</i>	-	-
	<i>O₂</i>	-	-
	<i>H₂</i>	917.6	917.6
	<i>EEMPA</i>	186,228	186,228
	<i>EEMPA+CO₂</i>	28,076.1	28,076.1
	<i>CH₃OH</i>	3,451.5	3,451.5
Temperature (°C)	133	133	
Pressure (bar)	24.5	25	
Design Data	Temperature	133 C	
	Pressure	25 bar	
Utility Requirements	Net Work Required: 2.1 kW		
Comments	See Process Flow Diagram		

Heat Exchanger			
Identification	Item	<i>Heat Exchanger</i>	Date. 3/30
	Item No.	<i>E-106</i>	By. AK
	No. Required	1	
Function	Interstage heater		
Operation	Continuous		
Materials Handled			
Stream ID		S-25	S-26
	Quantity (lb/hr)	220,489.8	220,489.8
	Mass Composition:		
	<i>CO₂</i>	-	-
	<i>N₂ + Ar</i>	-	-
	<i>H₂O</i>	1,874	1,874
	<i>NO_x</i>	-	-
	<i>SO_x</i>	-	-
	<i>O₂</i>	-	-
	<i>H₂</i>	917.6	917.6
	<i>EEMPA</i>	186,228	186,228
	<i>EEMPA+CO₂</i>	28,076.1	28,076.1
	<i>CH₃OH</i>	3,451.5	3,451.5
	Temperature (°C)	133	120
	Pressure (bar)	25	25
	Vapor Fraction	-	-
Design Data			
	Cross Sectional Area	1,181 ft ²	
	Overall Heat Transfer Coefficient	75 BTU/ °F-ft ² -hr	
Utility Requirements	445 lb/hr low pressure steam		
Comments	See Process Flow Diagram		

Flash Column					
Identification	Item	<i>Flash Column</i>		Date	3/30
	Item No.	T-101		By	MT
	No. Required	1			
Function	Separate hydrogen from EEMPA, methanol, and water				
Operation	Continuous				
Materials Handled Stream ID	Quantity (lb/hr)	S-27	S-28	S-31	
		175,228	623	174,605	
	Mass Composition:				
	<i>CH₃OH</i>	0.038	0.424	0.037	
	<i>CO₂</i>	-	-	-	
	<i>N₂ + Ar</i>	-	-	-	
	<i>H₂O</i>	0.022	0.077	0.021	
	<i>NO_x</i>	-	-	-	
	<i>SO_x</i>	-	-	-	
	<i>O₂</i>	-	-	-	
	<i>H₂</i>	0.002	0.494	2.73x10 ⁻⁵	
	<i>EEMPA</i>	0.939	0.005	0.941	
	<i>EEMPA+CO₂</i>	-	-	-	
	Temperature (°C)	120	120	120	
	Pressure (bar)	25	23.7	23.7	
Mass Vapor Fraction	0.123	1	0		
Design Data	Heat Duty	0 cal/sec			
	Pressure Drop	0.34 bar			
	Number of Phases	2			
	Diameter	4.79 ft			
	Height	19.18 ft			
Comments	See Process Flow Diagram and Appendix A				

Distillation Column 1					
Identification	Item	<i>Distillation Column</i>		Date	3/30
	Item No.	T-102		By	MT
	No. Required	1			
Function	Separate EEMPA from methanol and water				
Operation	Continuous				
Materials Handled Stream ID		S-31	S-33	S-45	S-42
	Quantity (lb/hr)	174,605	163,833	10,295	477
	Composition:				
	<i>CH₃OH</i>	0.037	4.73x10 ⁻⁹	0.629	0.889
	<i>CO₂</i>	-	-	-	-
	<i>N₂ + Ar</i>	-	-	-	-
	<i>H₂O</i>	0.021	2.59x10 ⁻⁵	0.371	0.092
	<i>NO_x</i>	-	-	-	-
	<i>SO_x</i>	-	-	-	-
	<i>O₂</i>	-	-	-	-
	<i>H₂</i>	2.73x10 ⁻⁵	1.28x10 ⁻³⁰	1.19x10 ⁻⁷	0.019
	<i>EEMPA</i>	0.941	1	2.04x10 ⁻²⁸	2.38x10 ⁻³⁴
	<i>EEMPA+CO₂</i>	-	-	-	-
	Temperature (°C)	120	139	10.2	10.2
	Pressure (bar)	23.7	0.087	0.067	0.067
Mass Vapor Fraction	0	0	0	1	
Design Data	Condenser Temperature	10.2 °C	Tower Diameter	4.26 m	
	Reboiler Temperature	189 °C	Tower Height	15.43 m	
	Tray Type	Sieve	Mass Reflux Ratio	3	
	Tray Spacing	0.61 m	Number of Stages	22	
	Number of Passes	2	Feed Stage	16	
Utility Requirements	Reboiler Heating Required	2,907,900 cal/sec			
	Condenser Heating Required	-2,103,790 cal/sec			
Comments	See Process Flow Diagram and Appendix A				

Partial Condenser			
Identification	Item	<i>Shell and Tube Heat Exchanger</i>	Date 3/30
	Item No.	E-108	By MT
	No. Required	1	
Function	Condense some of the vapor leaving the top of the distillation column		
Operation	Continuous		
Materials Handled Stream ID		S-40	S-41
	Quantity (lb/hr)	40,735	40,735
	Mass Composition:		
	<i>CH₃OH</i>	0.630	0.630
	<i>CO₂</i>	-	-
	<i>N₂ + Ar</i>	-	-
	<i>H₂O</i>	0.370	0.370
	<i>NO_x</i>	-	-
	<i>SO_x</i>	-	-
	<i>O₂</i>	-	-
	<i>H₂</i>	8.57×10^{-5}	8.57×10^{-5}
	<i>EEMPA</i>	0	0
	<i>EEMPA+CO₂</i>	-	-
	Temperature (°C)	29.6	10.2
Pressure (bar)	0.0689	0.0689	
Mass Vapor Fraction	1	0.004	
Design Data	Cross Sectional Area	11,634 ft ²	
	Overall Heat Transfer Coefficient	200 BTU/ °F-ft ² -hr	
Utility Requirements	479,341 lb/hr chilled water		
Comments	See Process Flow Diagram and Appendix A		

Reflux Drum				
Identification	Item	<i>Horizontal Vessel</i>		Date 3/30
	Item No.	V-100		By MT
	No. Required	1		
Function	Collect the condensed liquid for reflux back into the distillation column			
Operation	Continuous			
Materials Handled Stream ID		S-41	S-42	S-43
	Quantity (lb/hr)	40,735	183	40,552
	Composition:			
	<i>CH₃OH</i>	0.630	0.891	0.629
	<i>CO₂</i>	-	-	-
	<i>N₂ + Ar</i>	-	-	-
	<i>H₂O</i>	0.370	0.092	0.371
	<i>NO_x</i>	-	-	-
	<i>SO_x</i>	-	-	-
	<i>O₂</i>	-	-	-
	<i>H₂</i>	8.57×10^{-5}	0.019	1.23×10^{-7}
	<i>EEMPA</i>	0	0	0
	<i>EEMPA+CO₂</i>	-	-	-
	Temperature (°C)	10.2	10.2	10.2
	Pressure (bar)	0.0667	0.0667	0.0667
Mass Vapor Fraction	0.004	1	0	
Design Data	Holdup Time	5 minutes		
	Diameter	1.15 m		
	Length	3.44 m		
Comments	See Process Flow Diagram and Appendix A			

Kettle Reboiler			
Identification	Item	<i>Shell and Tube Heat Exchanger</i>	Date 3/30
	Item No.	E-107	By MT
	No. Required	1	
Function	Vaporize some of the stream leaving the bottom of the distillation column		
Operation	Continuous		
Materials Handled Stream ID		S-38	S-39
	Quantity (lb/hr)	163,539	163,539
	Composition:		
	<i>CH₃OH</i>	0	0
	<i>CO₂</i>	-	-
	<i>N₂ + Ar</i>	-	-
	<i>H₂O</i>	2.59×10^{-5}	2.59×10^{-5}
	<i>NO_x</i>	-	-
	<i>SO_x</i>	-	-
	<i>O₂</i>	-	-
	<i>H₂</i>	0	0
	<i>EEMPA</i>	1	1
	<i>EEMPA+CO₂</i>	-	-
	Temperature (°C)	139	189
	Pressure (bar)	0.087	0.087
Mass Vapor Fraction	0	1	
Design Data	Cross Sectional Area	1,462 ft ²	
	Overall Heat Transfer Coefficient	300 BTU/ °F-ft ² -hr	
Utility Requirements	4,190 lb/hr high pressure steam		
Comments	See Process Flow Diagram and Appendix A		

Pump			
Identification	Item	<i>Pump</i>	Date 3/30
	Item No.	P-104	By MT
	No. Required	1	
Function	Provide driving force for flow between distillation columns		
Operation	Continuous		
Materials Handled Stream ID		S-45	S-46
	Quantity (lb/hr)	10,149	10,149
	Composition:		
	<i>CH₃OH</i>	0.629	0.629
	<i>CO₂</i>	-	-
	<i>N₂ + Ar</i>	-	-
	<i>H₂O</i>	0.371	0.371
	<i>NO_x</i>	-	-
	<i>SO_x</i>	-	-
	<i>O₂</i>	-	-
	<i>H₂</i>	1.19x10 ⁻⁷	1.19x10 ⁻⁷
	<i>EEMPA</i>	2.04x10 ⁻²⁸	2.04x10 ⁻²⁸
	<i>EEMPA+CO₂</i>	-	-
	Temperature (°C)	10.5	11.0
Pressure (bar)	0.067	5.07	
Mass Vapor Fraction	0	0	
Design Data	Pressure Change	5 bar	
	Head Developed	59.3 m-kgf/kg	
Utility Requirements	Net Work Required	2.28 kW	
Comments	See Process Flow Diagram		

Distillation Column 2				
Identification	Item	<i>Distillation Column</i>	Date 3/28	
	Item No.	T-103	By MT	
	No. Required	1		
Function	Separate methanol and water			
Operation	Continuous			
Materials Handled Stream ID	Quantity (kg/hr)	S-46 10,149	S-55 6,362	S-48 3,787
	Composition:			
	<i>CH₃OH</i>	0.629	0.996	0.008
	<i>CO₂</i>	-	-	-
	<i>N₂ + Ar</i>	-	-	-
	<i>H₂O</i>	0.371	0.004	0.992
	<i>NO_x</i>	-	-	-
	<i>SO_x</i>	-	-	-
	<i>O₂</i>	-	-	-
	<i>H₂</i>	1.19x10 ⁻⁷	190 ppb	trace
	<i>EEMPA</i>	2.04x10 ⁻²⁸	0	0
	<i>EEMPA+CO₂</i>	-	-	-
	Temperature (°C)	11.0	94.9	128
	Pressure (bar)	5.07	3.00	3.00
Mass Vapor Fraction	0	0	0	
Design Data	Condenser Temperature	94.9 °C	Tower Diameter	1.04 m
	Reboiler Temperature	133 °C	Tower Height	21.1 m
	Tray Type	Sieve	Mass Reflux Ratio	3.22
	Tray Spacing	0.61 m	Number of Stages	30
	Number of Passes	2	Feed Stage	16
Utility Requirements	Reboiler Heating Required	950,476 cal/sec		
	Condenser Heating Required	-830,210 cal/sec		
Comments	See Process Flow Diagram and Appendix A			

Total Condenser			
Identification	Item	<i>Shell and Tube Heat Exchanger</i>	Date 3/30
	Item No.	E-110	By MT
	No. Required	1	
Function	Condense the methanol vapor leaving the top of the distillation column		
Operation	Continuous		
Materials Handled Stream ID	Quantity (lb/hr)	S-51 26,561	S-52 26,561
	Mass Composition:		
	<i>CH₃OH</i>	0.996	0.996
	<i>CO₂</i>	-	-
	<i>N₂ + Ar</i>	-	-
	<i>H₂O</i>	0.004	0.004
	<i>NO_x</i>	-	-
	<i>SO_x</i>	-	-
	<i>O₂</i>	-	-
	<i>H₂</i>	0	0
	<i>EEMPA</i>	0	0
	<i>EEMPA+CO₂</i>	-	-
	Temperature (°C)	95.2	94.9
	Pressure (bar)	3.00	3.00
Mass Vapor Fraction	1	0	
Design Data	Cross Sectional Area	582 ft ²	
	Overall Heat Transfer Coefficient	200 BTU/ °F-ft ² -hr	
Utility Requirements	257,833 lb/hr cooling water		
Comments	See Process Flow Diagram and Appendix A		

Reflux Drum			
Identification	Item	<i>Horizontal Vessel</i>	Date 3/30
	Item No.	V-101	By MT
	No. Required	1	
Function	Collect the condensed liquid for reflux back into the distillation column		
Operation	Continuous		
Materials Handled		S-52	S-53
Stream ID	Quantity (lb/hr)	26,561	26,561
	Mass Composition:		
	<i>CH₃OH</i>	0.996	0.996
	<i>CO₂</i>	-	-
	<i>N₂ + Ar</i>	-	-
	<i>H₂O</i>	0.004	0.004
	<i>NO_x</i>	-	-
	<i>SO_x</i>	-	-
	<i>O₂</i>	-	-
	<i>H₂</i>	0	0
	<i>EEMPA</i>	0	0
	<i>EEMPA+CO₂</i>	-	-
	Temperature (°C)	94.9	94.9
	Pressure (bar)	3.00	3.00
	Mass Vapor Fraction	0	0
Design Data	Holdup Time	5 minutes	
	Diameter	1.07 m	
	Length	3.21 m	
Comments	See Process Flow Diagram and Appendix A		

Kettle Reboiler			
Identification	Item	<i>Shell and Tube Heat Exchanger</i>	Date 3/30
	Item No.	E-109	By MT
	No. Required	1	
Function	Vaporize some of the stream leaving the bottom of the distillation column		
Operation	Continuous		
Materials Handled Stream ID		S-49	S-50
	Quantity (lb/hr)	14,861	14,861
	Composition:		
	<i>CH₃OH</i>	0.008	0.008
	<i>CO₂</i>	-	-
	<i>N₂ + Ar</i>	-	-
	<i>H₂O</i>	0.992	0.992
	<i>NO_x</i>	-	-
	<i>SO_x</i>	-	-
	<i>O₂</i>	-	-
	<i>H₂</i>	0	0
	<i>EEMPA</i>	0	0
	<i>EEMPA+CO₂</i>	-	-
	Temperature (°C)	128	133
Pressure (bar)	3.00	3.00	
Mass Vapor Fraction	0	1	
Design Data	Cross Sectional Area	436 ft ²	
	Overall Heat Transfer Coefficient	400 BTU/ °F-ft ² -hr	
Utility Requirements	1,603 lb/hr medium pressure steam		
Comments	See Process Flow Diagram and Appendix A		

19. Equipment Cost Summary

Table 19.1 Equipment Costs

Unit Type	Unit No.	Purchase Cost	Bare Module Factor	Bare Module Cost
Condenser	E-100	\$71,238	3.21	\$258,093
Condenser	E-101	\$55,897	3.21	\$201,189
Blower	C-100	\$2,561	3.21	\$8,224
Heater	E-102	\$23,991	3.21	\$77,011
Absorber	T-100	\$360,941	3.21	\$1,158,622
Pump	P-100	\$9,681	3.21	\$40,340
Intercooler	E-103	\$61,950	3.21	\$198,862
Pump	P-101	\$12,522	3.21	\$40,198
Intercooler	E-104	\$58,799	3.21	\$188,745
Pump	P-102	\$12,566	3.21	\$31,079
Heater	E-105	\$53,217	3.21	\$170,825
Reactor	R-100	\$28,120	3.21	\$90,266
Pump	P-103	\$3,579	3.21	\$250,382
Heater	E-106	\$40,119	3.21	\$128,782
Blower	C-101	\$3,161	3.21	\$10,148
Flash Column	T-101	\$95,918	3.21	\$307,899
Distillation Column	T-102	\$416,191	3.21	\$1,335,975
Reboiler	E-107	\$41,111	3.21	\$131,968
Partial Condenser	E-108	\$151,350	3.21	\$485,836
Reflux Drum	V-100	\$20,515	3.21	\$65,855
Pump	P-104	\$3,579	3.21	\$11,489
Distillation Column	T-103	\$121,928	3.21	\$391,389

Unit Type	Unit No.	Purchase Cost	Bare Module Factor	Bare Module Cost
Reboiler	E-109	\$27,490	3.21	\$88,243
Total Condenser	E-110	\$29,546	3.21	\$94,843
Reflux Drum	V-101	\$19,238	3.21	\$61,757

20. Fixed Capital Investment Summary

Fixed capital investment includes equipment costs, cost of catalyst, EEMPA, site preparation, service facilities, land, contingencies, contractor fees as well as cost of plant start-up.

The results of our calculations are reported in Table 20.1.

Table 20.1 Summary of Capital Investment

<u>Investment Summary</u>	
<u>Total Bare Module Costs:</u>	
Fabricated Equipment	\$ 4,976,878
Process Machinery	\$ 851,142
Catalysts	\$ 853,622
<u>Total Bare Module Costs:</u>	<u>\$ 6,681,642</u>
<u>Direct Permanent Investment</u>	
Cost of Site Preparations:	\$ 334,082
Cost of Service Facilities:	\$ 334,082
<u>Direct Permanent Investment</u>	<u>\$ 7,349,806</u>
<u>Total Depreciable Capital</u>	
Cost of Contingencies & Contractor Fees	\$ 1,322,965
<u>Total Depreciable Capital</u>	<u>\$ 8,672,771</u>
<u>Total Permanent Investment</u>	
Cost of Land:	\$ 173,455
Cost of Plant Start-Up:	\$ 867,277
<u>Total Permanent Investment</u>	<u>\$ 9,713,504</u>

21. Operating Costs - Costs of Manufacture

The cost of manufacture for the proposed process includes variable and fixed costs. Variable costs for the process include the cost of raw materials, byproducts, utilities and general expenses. The fixed costs for the process include the cost of operations, maintenance, operating overhead, property taxes and insurance. The summary of the incurred costs are presented in Table 21.1

Table 21.1: Summary of Operating Costs

Variable Cost Summary			
<u>Variable Costs at 100% Capacity:</u>			
<u>General Expenses</u>			
	Selling / Transfer Expenses:		\$ 494,709
	Direct Research:		\$ 791,534
	Allocated Research:		\$ 82,451
	Administrative Expense:		\$ 329,806
	Management Incentive Compensation:		\$ 206,129
	Total General Expenses		\$ 1,904,628
<u>Raw Materials</u>	\$0.136034	per lb of Methanol	\$6,924,517
<u>Byproducts</u>	\$0.022636	per lb of Methanol	(\$1,152,212)
<u>Utilities</u>	\$0.061530	per lb of Methanol	\$3,132,057
	<u>Total Variable Costs</u>		<u>\$ 10,808,991</u>
Fixed Cost Summary			
<u>Operations</u>			
	Direct Wages and Benefits		\$ 416,000
	Direct Salaries and Benefits		\$ 62,400

Operating Supplies and Services	\$	24,960
Technical Assistance to Manufacturing	\$	300,000
Control Laboratory	\$	325,000
Total Operations	\$	1,128,360

Maintenance

Wages and Benefits	\$	390,275
Salaries and Benefits	\$	97,569
Materials and Services	\$	390,275
Maintenance Overhead	\$	19,514
Total Maintenance	\$	897,632

Operating Overhead

General Plant Overhead:	\$	68,603
Mechanical Department Services:	\$	23,190
Employee Relations Department:	\$	57,008
Business Services:	\$	71,502
Total Operating Overhead	\$	220,303

Property Taxes and Insurance

Property Taxes and Insurance:	\$	173,455
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Total Fixed Costs **\$ 2,419,751**

Table 21.1 summarizes the raw material costs for manufacturing methanol. It can be seen that Hydrogen makes 80% of the cost and the rest 20% is attributed to EEMPA replenishment. Future, cost reductions would focus on reducing EEMPA replenishment rate or finding cheaper sources of Hydrogen.

Table 21.1: Summary of Raw Material Costs

Raw Material:	Required Ratio:		Cost of Raw Material:	%
Hydrogen	0.19	lb per lb of Methanol	\$0.11	81%
EEMPA Replenishment	0.01	lb per lb of Methanol	\$0.03	19%

22. Other Important Considerations

22.1 Location

The planned location for this proposed carbon capture project is the southeastern, Gulf Coast region of the United States. Around the Gulf Coast there are many coal fired power plants in operation which would provide ample amounts of flue gas to supply our process. Additionally, an extensive system of hydrogen pipelines spans the Gulf Coast region which will allow for convenient access to hydrogen for the hydrogenation reaction. Figure 22.1 shows the numerous coal fired power plants within the Gulf Coast region, and seen in Figure 22.2, there is an easily accessible hydrogen pipeline that runs through the region as well. Considering both figures simultaneously in Figure 22.1, it can be seen that the close proximity of the coal fired power plants to the hydrogen pipeline makes this the ideal location to host our process.

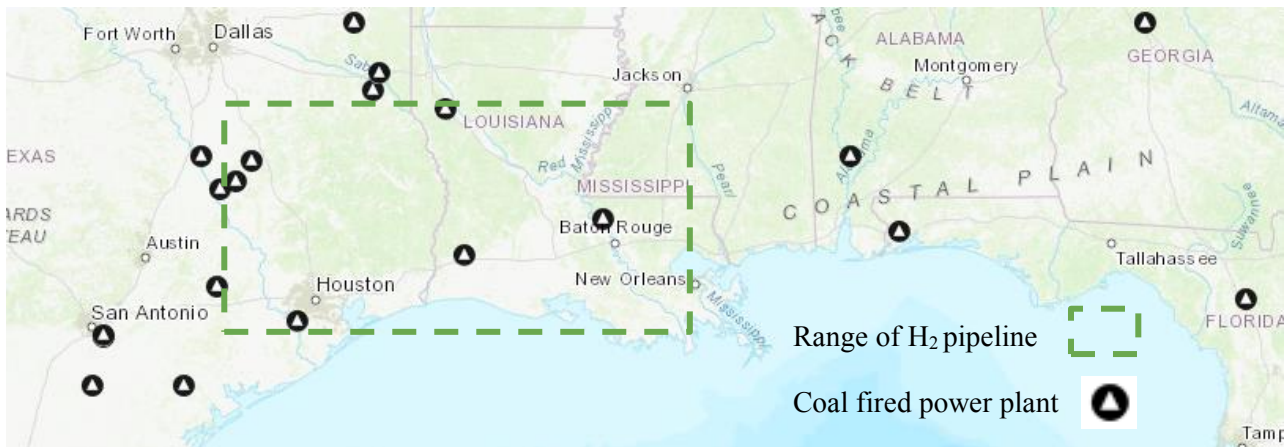


Figure 22.1. This map shows the locations of coal fire plants in existence in the Gulf Coast. The segment highlighted by the box matches the region covered by the hydrogen pipeline shown in Figure below (US Energy Information Administration, n.d.).



Figure 22.2 The map above shows Air Products' extensive Gulf Coast Hydrogen pipeline system. It is the world's largest hydrogen pipeline and reaches over 600 miles, stretching from Houston to New Orleans (Air Products, 2012).

22.2 Environmental Factors

The main goal of our carbon capture and utilization process is to reduce the amount of CO₂ emissions into the atmosphere in order to slow and reverse climate change. While our process is carbon negative and avoids the carbon heavy emissions sourced from the production of methanol by natural gas reforming, there are still many points along the life cycle of our process that leads to CO₂ emissions. To maximize environmental benefits, ideally, we would utilize green hydrogen for our hydrogenation reaction and we would supply all of our energy needs with energy from renewable resources. With the cost of renewable energy decreasing due to new technological advancements, this option has lots of potential in the coming years. However, with the high cost of green hydrogen, it will be difficult to incorporate it into our reaction without significant additional financial support from subsidies.

By bringing so many benefits to the environmental health of the atmosphere, carbon capture's impacts on other regions of the environment are often overlooked yet have been found in some studies to produce negative consequences. With limited experimental data available on EEMPA, studies done on similar amine-based scrubbing solvents can be used as an indicator for the potential harms to look out for when working with EEMPA. With monoethanol amine (MEA), the potential for photochemical oxidant formation increased from levels of coal fired power plants to power plants with carbon capture. Photochemical oxidants include ozone which can lead to lung damage among humans and can cause significant harm to sensitive vegetation and ecosystems, especially during the growing season. However, the decreases seen in particulate matter, terrestrial and aquatic toxicity, human toxicity, and terrestrial acidification indicate that various aspects of environmental damage seen from coal fired power plants can be mitigated with the incorporation of carbon capture (Veltman et al., 2010). For MEA, the maximum amount of tolerable emissions

was found to be 12 t/year, above which, toxicity to aquatic systems becomes a major concern (Karl et al., 2011). With several freshwater lakes along the region we plan to base our process, concerns over these aquatic ecosystems are critically important, so extra monitoring and care will be taken during operation to minimize harm to the greatest extent possible.

Care must be taken with the collection and treatment of the EEMPA exiting our process through the purge stream as the degradation products pose potential environmental threats (Veltman et al., 2010). It has been assumed that EEMPA's degradation products are mobile in aquatic ecosystems and are not decomposed in soil or water, so any harms have far reaching potential (Karl et al., 2011). To ensure the smallest environmental impact, EEMPA and its degradation products will be handled with extreme care to avoid spills, leaks, or emissions into the uncontrolled, surrounding environment.

As more studies and data on EEMPA become available, the extent of environmental impacts will be revisited to ensure the process is not only benefiting the atmosphere by the reduction of CO₂ emissions, but also ensuring the protection of the surrounding terrestrial and aquatic life impacted by the process.

The flue gas used as the carbon source for the process will be treated with desulfurization equipment, also known as scrubbers, to reduce the quantity of incoming SO_x. These scrubbers have also been found to successfully reduce the amount of NO_x and mercury emissions in the flue gas as well. Limiting the amount of NO_x and SO_x emissions is beneficial as these compounds contribute greatly to climate change, the depletion of the ozone layer in the troposphere, and are harmful to human health. Reducing the incoming concentration of NO_x and SO_x is also beneficial for the success and safety of the process as SO₂ and NO₂ can react with EEMPA, causing oxidative degradation (Veltman et al., 2010).

Additionally, care will be taken to ensure our plant is compliant with all regulations set forth by the Environmental Protection Agency (EPA), including those outlined in The Clean Air Act, The Clean Water Act, and any other policies pertaining to our planned project.

22.3 Public and Employee Safety, Health, and Welfare

The safety, health, and welfare of all of our staff and employees is our top priority. In order to ensure the safest workspace as possible, each new member of our team will undergo rigorous safety training to allow for an in-depth understanding of all of the risks and hazards associated with the equipment and chemicals used in the workplace. A review of this training will be revisited by all returning employees annually. All chemicals and equipment in the workplace will be clearly and accurately labeled to avoid misuse and to provide safety and emergency information. Eating, drinking, and smoking is prohibited where any and all chemicals are handled, stored, or processed.

The flue gas to be treated in our process will enter the system at 57°C and 15 psia. The flue gas will run through a desulfurization system prior to entering the process to reduce the amount of NO_x and SO_x emitted in the air and within the system. Despite the low concentration of NO_x and SO_x in our source of flue gas, care must be taken by employees to ensure the flue gas is approached and handled safely. Inhalation of NO_x and SO_x can lead to short- and long-term respiratory challenges, and at high temperatures, the flue gas may cause burns. Nitrogen and argon make up the largest portion of the incoming flue gas stream and although inert and nontoxic, both are simple asphyxiants that can lead to suffocation upon the displacement of oxygen. Carbon dioxide is deemed hazardous by the Occupational Safety and Health Administration (OSHA) Hazard Communication Standard. As a gas under high pressures, it may explode if heated and upon the displacement of oxygen, it can cause rapid suffocation, increased heart rate, or respiration.

Not many full life-cycle and environmental, health, and safety hazard assessments have been conducted on new post-combustion carbon capture solvents, however, leaning on studies done with reference systems, we can estimate the best practices for handling EEMPA safely. Concerns have risen over the carcinogenic and toxic properties of the nitrosamines and nitramines

produced during amine solvent degradation, however if kept below 13.7-14 mM, these will pose a minimal threat to human health. With EEMPA's relatively high boiling point of 181°C, the solvent is less mobile than alternative carbon capture solvents and is therefore a lower threat to human health and safety. As with all potentially harmful chemicals, it will be required that EEMPA be handled with care to avoid contact with eyes and skin and to avoid inhalation of any fumes. Although EEMPA degradation products are not well researched, they have the potential to exhibit carcinogenic or toxic properties and thus all flows of EEMPA, especially the recycle and purge streams, should be safely controlled and their contents experimentally identified through further research (Shavaliyeva et al., 2021).

Hydrogen is also considered hazardous by OSHA standards as it is an extremely flammable gas that may explode under pressure if heated. Hydrogen can cause suffocation by the rapid displacement of oxygen, and burns with an invisible flame, making fires difficult to detect. In order to avoid hazards, all pipelines containing hydrogen will be placed in cool, dry spaces and away from direct sunlight or ignition sources (see Appendix D).

Methanol is a highly flammable substance and is toxic if swallowed, inhaled, or if it comes in contact with skin. Following a single exposure to methanol can result in damage to organs. Due to its flammability, the methanol produced will be stored in a cool place, in a tightly sealed container and away from any extreme heat, ignition sources, or open flames (see Appendix D). Methanol flames are not clearly visible in direct sunlight, so early spill or leakage detection, immediate response, and appropriate action are imperative (Medina, 2014).

All workers involved with or near the handling and processing of chemicals will be required to wear all of the necessary and proper personal protective equipment (PPE), including protective gloves, clothing, and eye protection. All plant operation zones containing or purposed

for handling hazardous chemicals or substances will be locked and fenced off accordingly with appropriate warning signs. Only those with proper safety training and PPE will be granted access to these zones.

As an organization we commit to equal opportunity and equitable pay for all of our hires and employees. Any discrimination or harassment of any kind, especially that pertaining to race, religion, age, sex, national origin, disability status, protected veteran status, sexual orientation, gender identity or expression, or any other identity is strictly prohibited in and outside of the workplace.

22.4 Global, Cultural, Societal, and Ethical Factors

While carbon capture and utilization can go a long way in reducing current CO₂ emission rates, we remain conscious that the best way to address the climate emergency is to stop the production of CO₂ emissions all together. Perfecting the technology of carbon capture is risky because it may lead to the belief that it can be used as a total solution to the climate crisis, enticing people and corporations to resume their current rates of fossil fuel consumption. Instead, CCS and CCU projects are to be used as a supplement to the efforts to reduce emissions. It is our hope that these supplements will allow us as a society to obtain extra time for the research and development of new technologies to replace the ones responsible for emitting CO₂, before climate change intensifies beyond the point of no return.

Although this project will not be economically viable without financial government assistance, each newly designed process brings all carbon capture technology one step forward. Each design is a learning experience to bring cost cutting and efficient innovations to the technology, making each project more feasible for future endeavors (TED, 2018).

Although the emissions from our process are not predicted to cause significant damage or harm to human health, it is crucial to ensure there are no surrounding communities that are threatened or disturbed by our CCU process. Presently and throughout history, low-income communities and communities of color are often the first to be impacted by harmful emissions and acts of environmental injustice. In the specific siting of our process we need to be conscious and mindful of this reality in order to avoid placing a burden on the health and livelihood of any and all communities.

Nearby our planned plant location along the Gulf Coast region of the southeastern US, there are several Indian reservations in Texas and Louisiana. The Alabama-Coushatta, Tunica-

Biloxi, Chitimacha, and Coushatta lands will be left undisturbed by the realization of our carbon capture process and no unwarranted pipelines or any transportation of materials we use will run on, under, or through their lands.



Figure 22.3 Map of Indian lands of federally recognized tribes of the US. Nearby the planned location of our carbon capture process are the Alabama-Coushatta, Tunica-Biloxi, Chitimacha, and Coushatta lands (Bureau of Indian Affairs, 2016).

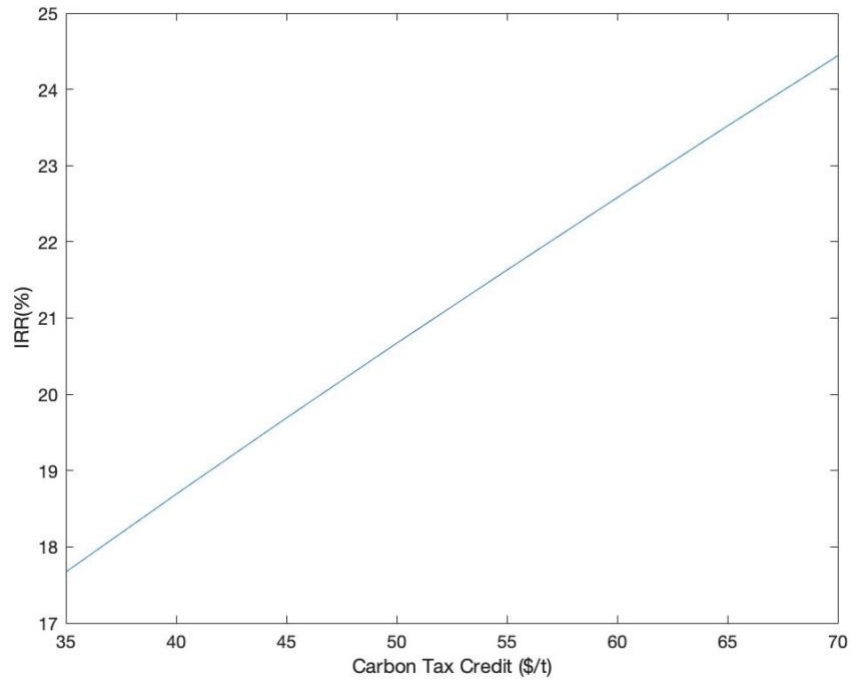
22. Profitability Analysis

Table 23.1 summarizes the profitability parameters for the proposed plant. The following profitability is based on selling price of \$0.32/lb methanol and \$35/ton CO₂ absorbed carbon tax credit. The market price of bulk methanol is \$0.22/lb methanol; however the traditional manufacturing process to produce methanol adds 1-3 tons of CO₂ per ton of methanol to the environment while our “green methanol” even after utilizing H₂ is an overall net-carbon negative product (absorbs 0.9 tons CO₂ per ton of methanol), which creates an incentive for companies to pay an additional amount to offset their carbon emissions.

Table 23.1 ROI Analysis

Annual Sales	\$ 15,440,847
Annual Costs	\$ (12,638,615)
Depreciation	\$ (777,080)
Income Tax	\$ (465,785)
Net Earnings	\$ 1,559,367
Total Capital Investment	\$ 10,796,897
ROI	14.44%
Internal Rate of Return	17.67%
Net Present Value (NPV) at Cost of Capital 15%	\$ 1,441,800

Currently the project is estimated to run at an internal rate of investment (IRR) of 17.67%. There are two main pathways to make a more profitable project at this point. The first would be to increase the carbon tax credit beyond its current projection. Analyzing the 45Q tax credit in the appendix, the current projection for when the plant will be built is 35\$/t for utilization. For reference, currently in 2021 United Kingdoms has a tax credit of 22\$/t, France 49\$/t and Sweden 119\$/t, while the US has 20\$/ton in 2020. The second pathway to profitability is to increase the selling price of methanol. The current market price for methanol, according to Methanex, is \$0.22/lb. A “green” premium could be charged for the methanol allowing for higher selling prices, however the level of “green” can vary based on how the hydrogen is sourced. The project designed here produces methanol with significantly less carbon dioxide produced compared to usual methanol production, however the hydrogen is sourced in the cheapest way, which involves the use of fossil fuels. Usual production of methanol produces 0.7-1.0t of CO₂ per 1t of methanol using natural gas and 3t of CO₂ per 1t of methanol using coal gasification. The system designed here consumes 0.9t of CO₂ per 1t of methanol produced (CRI). Switching to more green forms of hydrogen would further increase this consumption number. According to a report by the Netherlands Ministry of Economics green methanol is proposed to sell for in between \$0.27/lb and \$0.31/lb. The following sensitivity graph shows the relationship between carbon tax and IRR.



The desired range of carbon tax credits starts at 35\$/t, which is the projected amount at the start of construction and ranges up to 70\$/t which is a relatively large increase but is realistic when comparing to European countries. According to McKinsey & Company the average IRR for chemical products range from 18% to 23%. At a carbon tax credit of 35\$/t, this project is slightly below the range and surpasses at a tax credit of 40\$/t.

23. Conclusions and Recommendations

The process designed effectively captures carbon dioxide, using the proprietary binding organic liquid EEMPA, and converts it into methanol. The design contains the major operations including binding the carbon dioxide into EEMPA, hydrogenating the bound carbon dioxide into methanol using hydrogen, and separating out the methanol using distillation. Due to the proprietary nature of EEMPA, assumptions were made when it comes to important variables such as mass transfer coefficients and kinetics. As more data becomes available on EEMPA, a more rigorous evaluation can be made on its effectiveness and profitability when it comes to the conversion of carbon dioxide into methanol.

The project consumes 0.9t of carbon dioxide per 1t of methanol produced as thus is carbon negative. This paired with an aggressive carbon tax credit plan and increasing prices of green methanol could lead to a profitable investment. The precedent is set as countries in Europe have shown the ability to have a working large carbon tax credit and as climate mitigation policies continue, the price of green methanol should only increase. Further optimization of the design, in terms of heat integration and capital and operating costs, could lead to lower costs and thus hydrogen could be sourced in a more carbon neutral way. This would further increase the plants carbon consumption and in turn the premium applied to the methanol selling price. As more research is carried out on EEMPA and its interactions with carbon dioxide and other useful products, a more robust optimization of the economics can be made.

24. Acknowledgements

As a team, we would like to extend our greatest appreciation to our project author, Dr. Matthew Targett for providing us with an abundance of contacts, resources, and insights to aid in our success. Thank you to Dr. Talid Sinno, our project advisor, for assisting and guiding us every step of the way. We would also like to give a special thanks to Professor Bruce Vrana for his continual support of our team and our peers throughout the entire senior design process. We appreciate all the time and consideration Professor Leonard Fabiano gave to our group, who was an immense help in the construction of our process simulation. Additional thanks go out to all of the industrial consultants that aided us along the way week after week. Their respectful feedback and experience were essential factors in making this project possible. We would also like to acknowledge the University of Pennsylvania's entire Department of Chemical and Biomolecular Engineering for engaging with us in an open, effective learning environment and mentoring us and our peers throughout our time in the program.

During such a tumultuous time in the world, all of our consultants, professors, and advisors were there to provide us with the resources and support necessary to make the most out of a challenging situation. Each member of our team learned and gained so much from this experience and we are forever grateful to have been granted such an empowering opportunity.

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Exceptionally Low Operational Heat and Total Costs of Capture - Comprehensive
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26. Appendix A: Miscellaneous Calculations

Aspen Plus Simulation Report

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PLATFORM: WIN-X64                        APRIL 15, 2021
VERSION: 37.0   Build 396 Patchlevel 1   THURSDAY
INSTALLATION:                               10:32:39 P.M.

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ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE I

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TABLE OF CONTENTS

RUN CONTROL SECTION.....	1
RUN CONTROL INFORMATION.....	1
FLOWSHEET SECTION.....	2
FLOWSHEET CONNECTIVITY BY STREAMS.....	2
FLOWSHEET CONNECTIVITY BY BLOCKS.....	2
COMPUTATIONAL SEQUENCE.....	2
OVERALL FLOWSHEET BALANCE.....	2
PHYSICAL PROPERTIES SECTION.....	3
COMPONENTS.....	3
U-O-S BLOCK SECTION.....	4

BLOCK: FLASH	MODEL: FLASH2.....	4
BLOCK: NRTLDIST	MODEL: RADFRAC.....	5
BLOCK: PUMP	MODEL: PUMP.....	13
BLOCK: RADFRAC	MODEL: RADFRAC.....	14
STREAM SECTION.....		23
BTM FEED FLASHLIQ FLASHVAP LIQOVHD.....		23
METHANOL S-13 VAPOVHD WATER.....		24
PROBLEM STATUS SECTION.....		25
BLOCK STATUS.....		25

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE 1

RUN CONTROL SECTION

RUN CONTROL INFORMATION

THIS COPY OF ASPEN PLUS LICENSED TO UNIVERSITY OF PENNSYLVAN

TYPE OF RUN: NEW

INPUT FILE NAME: _4511wbz.inm

OUTPUT PROBLEM DATA FILE NAME: _3229hcs
LOCATED IN:

PDF SIZE USED FOR INPUT TRANSLATION:
NUMBER OF FILE RECORDS (PSIZE) = 0
NUMBER OF IN-CORE RECORDS = 256
PSIZE NEEDED FOR SIMULATION = 1

CALLING PROGRAM NAME: apmain
LOCATED IN: C:\Program Files\AspenTech\Aspen Plus V11.0\Engine\XeQ

SIMULATION REQUESTED FOR ENTIRE FLOWSHEET

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE 2

FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY STREAMS

STREAM	SOURCE	DEST	STREAM	SOURCE	DEST
FEED	----	FLASH	VAPOVHD	RADFRAC	----
LIQOVHD	RADFRAC	PUMP	BTM	RADFRAC	----
S-13	PUMP	NRTLDIST	METHANOL	NRTLDIST	----
WATER	NRTLDIST	----	FLASHVAP	FLASH	----
FLASHLIQ	FLASH	RADFRAC			

FLOWSHEET CONNECTIVITY BY BLOCKS

```

-----
BLOCK          INLETS          OUTLETS
RADFRAC        FLASHLIQ        VAPOVHD LIQOVHD BTM
PUMP           LIQOVHD          S-13
NRTLDIST       S-13             METHANOL WATER
FLASH          FEED             FLASHVAP FLASHLIQ

```

COMPUTATIONAL SEQUENCE

```

-----
SEQUENCE USED WAS:
  FLASH RADFRAC PUMP NRTLDIST

```

OVERALL FLOWSHEET BALANCE

```

-----
*** MASS AND ENERGY BALANCE ***
              IN              OUT              RELATIVE DIFF.
CONVENTIONAL COMPONENTS (KMOL/HR )
  WATER              95.0000              95.0000              0.614458E-07
  METHANOL           95.0000              95.0000              0.882237E-07
  H2                  71.0000              71.0000              0.195529E-08
  1-DOD-01           346.000              346.000              -0.414954E-07
TOTAL BALANCE
  MOLE (KMOL/HR )    607.000              607.000              0.00000
  MASS (KG/HR )      79078.1              79078.1              -0.341955E-07
  ENTHALPY (CAL/SEC ) -0.153099E+08        -0.143850E+08        -0.604134E-01

```

```

*** CO2 EQUIVALENT SUMMARY ***
FEED STREAMS CO2E          0.00000          KG/HR
PRODUCT STREAMS CO2E       0.00000          KG/HR
NET STREAMS CO2E PRODUCTION 0.00000          KG/HR
UTILITIES CO2E PRODUCTION  0.00000          KG/HR
TOTAL CO2E PRODUCTION      0.00000          KG/HR

```

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE 3

PHYSICAL PROPERTIES SECTION

COMPONENTS

```

-----
ID      TYPE  ALIAS      NAME
WATER   C      H2O        WATER
METHANOL C      CH4O       METHANOL
H2      C      H2         HYDROGEN
1-DOD-01 C      C14H30O-N18 1-DODECANOL,-2,2-DIMETHYL-

```

```

LISTID      SUPERCRITICAL COMPONENT LIST
HC-1        H2

```

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE 4

U-O-S BLOCK SECTION

BLOCK: FLASH MODEL: FLASH2

 INLET STREAM: FEED
 OUTLET VAPOR STREAM: FLASHVAP
 OUTLET LIQUID STREAM: FLASHLIQ
 PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
 HENRY-COMPS ID: HC-1

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE (KMOL/HR)	607.000	607.000	0.00000
MASS (KG/HR)	79078.1	79078.1	0.00000
ENTHALPY (CAL/SEC)	-0.153099E+08	-0.153099E+08	-0.649004E-10

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	0.00000	KG/HR
PRODUCT STREAMS CO2E	0.00000	KG/HR
NET STREAMS CO2E PRODUCTION	0.00000	KG/HR
UTILITIES CO2E PRODUCTION	0.00000	KG/HR
TOTAL CO2E PRODUCTION	0.00000	KG/HR

*** INPUT DATA ***

TWO PHASE PQ FLASH
 PRESSURE DROP BAR 0.34474
 SPECIFIED HEAT DUTY CAL/SEC 0.0
 MAXIMUM NO. ITERATIONS 30
 CONVERGENCE TOLERANCE 0.000100000

*** RESULTS ***

OUTLET TEMPERATURE C 119.99
 OUTLET PRESSURE BAR 24.655
 VAPOR FRACTION 0.12300

V-L PHASE EQUILIBRIUM :

COMP	F(I)	X(I)	Y(I)	K(I)
WATER	0.15651	0.17628	0.15533E-01	0.88115E-01
METHANOL	0.15651	0.17168	0.48337E-01	0.28156
H2	0.11697	0.20975E-02	0.93605	446.26
1-DOD-01	0.57002	0.64995	0.84674E-04	0.13028E-03

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE 5

U-O-S BLOCK SECTION

BLOCK: NRTLDIST MODEL: RADFRAC

 INLETS - S-13 STAGE 8
 OUTLETS - METHANOL STAGE 1

WATER STAGE 14
 PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
 HENRY-COMPS ID: HC-1

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE (KMOL/HR)	182.425	182.425	0.00000
MASS (KG/HR)	4536.17	4536.17	0.406204E-08
ENTHALPY (CAL/SEC)	-0.320116E+07	-0.308090E+07	-0.375695E-01

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	0.00000	KG/HR
PRODUCT STREAMS CO2E	0.00000	KG/HR
NET STREAMS CO2E PRODUCTION	0.00000	KG/HR
UTILITIES CO2E PRODUCTION	0.00000	KG/HR
TOTAL CO2E PRODUCTION	0.00000	KG/HR

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE 6

U-O-S BLOCK SECTION

BLOCK: NRTLDIST MODEL: RADFRAC (CONTINUED)

 **** INPUT DATA ****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	14
ALGORITHM OPTION	STANDARD
ABSORBER OPTION	NO
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	BROYDEN
DESIGN SPECIFICATION METHOD	NESTED
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	45
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	30
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

**** COL-SPECS ****

MOLAR VAPOR DIST / TOTAL DIST	0.0
MASS REFLUX RATIO	3.00000
MASS DISTILLATE RATE	KG/HR 3,100.00

**** PROFILES ****

P-SPEC	STAGE 1 PRES, BAR	3.00000
--------	-------------------	---------

 **** RESULTS ****

*** COMPONENT SPLIT FRACTIONS ***

COMPONENT:	OUTLET STREAMS	
	METHANOL	WATER
WATER	.67859E-02	.99321
METHANOL	.99500	.50007E-02
H2	1.0000	0.0000

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE 7

U-O-S BLOCK SECTION

BLOCK: NRTLDIST MODEL: RADFRAC (CONTINUED)

*** SUMMARY OF KEY RESULTS ***

TOP STAGE TEMPERATURE	C	94.9288
BOTTOM STAGE TEMPERATURE	C	132.531
TOP STAGE LIQUID FLOW	KMOL/HR	287.903
BOTTOM STAGE LIQUID FLOW	KMOL/HR	93.1402
TOP STAGE VAPOR FLOW	KMOL/HR	0.0
BOILUP VAPOR FLOW	KMOL/HR	364.156
MOLAR REFLUX RATIO		3.22456
MOLAR BOILUP RATIO		3.90977
CONDENSER DUTY (W/O SUBCOOL)	CAL/SEC	-830,210.
REBOILER DUTY	CAL/SEC	950,476.

**** MANIPULATED VARIABLES ****

CALCULATED	BOUNDS			VALUE
	LOWER	UPPER		
MASS REFLUX RATIO	0.10000	5.0000		3.2246
MASS DISTILLATE RATE	KG/HR	100.00	3500.0	2852.0

**** DESIGN SPECIFICATIONS ****

NO	SPEC-TYPE	QUALIFIERS	UNIT	SPECIFIED VALUE	CALCULATED VALUE
1	MASS-FRAC	STREAMS: METHANOL		0.99600	0.99600
		COMPS: METHANOL			
2	MASS-RECOV	STREAMS: METHANOL		0.99500	0.99500
		COMPS: METHANOL			

**** MAXIMUM FINAL RELATIVE ERRORS ****

DEW POINT 0.22340E-04 STAGE= 8
 BUBBLE POINT 0.11061E-03 STAGE= 11
 COMPONENT MASS BALANCE 0.68619E-06 STAGE= 8 COMP=WATER
 ENERGY BALANCE 0.19098E-03 STAGE= 12

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE 8

U-O-S BLOCK SECTION

BLOCK: NRTLDIST MODEL: RADFRAC (CONTINUED)

**** PROFILES ****

NOTE REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS FROM THE STAGE INCLUDING ANY SIDE PRODUCT.

STAGE	TEMPERATURE C	PRESSURE BAR	ENTHALPY CAL/MOL		HEAT DUTY CAL/SEC
			LIQUID	VAPOR	
1	94.929	3.0000	-55209.	-47044.	-.83021+06
2	95.184	3.0000	-55293.	-47285.	
7	98.258	3.0000	-57442.	-48126.	
8	100.45	3.0000	-58858.	-48672.	
9	101.06	3.0000	-59234.	-48818.	
10	102.64	3.0000	-60160.	-49183.	
13	128.00	3.0000	-65972.	-55133.	
14	132.53	3.0000	-66158.	-56528.	.95048+06

STAGE	FLOW RATE KMOL/HR		FEED RATE KMOL/HR			PRODUCT RATE KMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	377.2	0.000				89.2845	
2	287.5	377.2					
7	274.3	368.9					
8	501.6	363.6	182.4247				
9	497.7	408.5					
10	488.5	404.6					
13	457.3	362.0					
14	93.14	364.2				93.1401	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE KG/HR		FEED RATE KG/HR			PRODUCT RATE KG/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.1205E+05	0.000				2851.9777	
2	9153.	0.1205E+05					
7	8022.	0.1133E+05					
8	0.1382E+05	0.1087E+05	4536.1740				
9	0.1348E+05	0.1213E+05					
10	0.1268E+05	0.1180E+05					

13 8425. 7421.
 14 1684. 6741.

1684.1962

ASPEN PLUS PLAT: WIN-X64 VER: 37.0

04/15/2021 PAGE 9

U-O-S BLOCK SECTION

BLOCK: NRTLDIST MODEL: RADFRAC (CONTINUED)

**** MOLE-X-PROFILE ****

STAGE	WATER	METHANOL	H2
1	0.70932E-02	0.99290	0.31028E-05
2	0.14640E-01	0.98536	0.21974E-08
7	0.19925	0.80075	0.41889E-09
8	0.32101	0.67899	0.34774E-09
9	0.35334	0.64666	0.18328E-12
10	0.43325	0.56675	0.82172E-16
13	0.97084	0.29163E-01	0.17748E-27
14	0.99522	0.47836E-02	0.10128E-31

**** MOLE-Y-PROFILE ****

STAGE	WATER	METHANOL	H2
1	0.34219E-02	0.99223	0.43483E-02
2	0.70932E-02	0.99290	0.31028E-05
7	0.94945E-01	0.90505	0.75125E-06
8	0.15206	0.84794	0.76230E-06
9	0.16728	0.83272	0.42702E-09
10	0.20557	0.79443	0.22547E-12
13	0.82276	0.17724	0.33896E-23
14	0.96460	0.35399E-01	0.22287E-27

**** K-VALUES ****

STAGE	WATER	METHANOL	H2
1	0.48242	0.99932	1401.4
2	0.48450	1.0077	1412.0
7	0.47661	1.1302	1793.0
8	0.47377	1.2488	2192.3
9	0.47354	1.2876	2328.9
10	0.47450	1.4017	2743.9
13	0.84747	6.0777	19100.
14	0.96924	7.3999	22006.

**** MASS-X-PROFILE ****

STAGE	WATER	METHANOL	H2
1	0.40005E-02	0.99600	0.19582E-06
2	0.82843E-02	0.99172	0.13914E-09
7	0.12273	0.87727	0.28872E-10
8	0.20999	0.79001	0.25454E-10
9	0.23501	0.76499	0.13640E-13
10	0.30060	0.69940	0.63797E-17
13	0.94928	0.50718E-01	0.19419E-28
14	0.99152	0.84766E-02	0.11291E-32

**** MASS-Y-PROFILE ****

STAGE	WATER	METHANOL	H2
1	0.19347E-02	0.99779	0.27510E-03
2	0.40005E-02	0.99600	0.19582E-06
7	0.55697E-01	0.94430	0.49313E-07
8	0.91591E-01	0.90841	0.51379E-07
9	0.10149	0.89851	0.28988E-10
10	0.12701	0.87299	0.15588E-13
13	0.72299	0.27701	0.33329E-24
14	0.93873	0.61272E-01	0.24270E-28

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE 10

U-O-S BLOCK SECTION

BLOCK: NRTLDIST MODEL: RADFRAC (CONTINUED)

 ***** HYDRAULIC PARAMETERS *****

*** DEFINITIONS ***

MARANGONI INDEX = SIGMA - SIGMATO
 FLOW PARAM = (ML/MV)*SQRT(RHOV/RHOL)
 QR = QV*SQRT(RHOV/(RHOL-RHOV))
 F FACTOR = QV*SQRT(RHOV)

WHERE:

SIGMA IS THE SURFACE TENSION OF LIQUID FROM THE STAGE
 SIGMATO IS THE SURFACE TENSION OF LIQUID TO THE STAGE
 ML IS THE MASS FLOW OF LIQUID FROM THE STAGE
 MV IS THE MASS FLOW OF VAPOR TO THE STAGE
 RHOL IS THE MASS DENSITY OF LIQUID FROM THE STAGE
 RHOV IS THE MASS DENSITY OF VAPOR TO THE STAGE
 QV IS THE VOLUMETRIC FLOW RATE OF VAPOR TO THE STAGE

TEMPERATURE

STAGE	C	
	LIQUID FROM	VAPOR TO
1	94.929	95.184
2	95.184	95.375
7	98.258	100.45
8	100.45	101.06
9	101.06	102.64
10	102.64	106.81
13	128.00	132.53
14	132.53	132.53

STAGE	MASS FLOW KG/HR		VOLUME FLOW L/MIN		MOLECULAR WEIGHT	
	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO

1	12048.	12048.	285.31	64173.	31.943	31.943
2	9152.8	12005.	216.65	64136.	31.837	31.862
7	8022.0	10874.	186.19	62740.	29.247	29.909
8	13815.	12131.	315.21	70610.	27.539	29.696
9	13481.	11797.	306.00	70226.	27.086	29.159
10	12683.	10999.	283.84	69382.	25.965	27.822
13	8425.4	6741.2	160.87	68238.	18.424	18.512
14	1684.2	0.0000	31.883	0.0000	18.082	

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE 11

U-O-S BLOCK SECTION

BLOCK: NRTLDIST MODEL: RADFRAC (CONTINUED)

STAGE	DENSITY GM/CC		VISCOSITY CP		SURFACE TENSION DYNE/CM	
	LIQUID	FROM VAPOR TO	LIQUID	FROM VAPOR TO	LIQUID	FROM
1	0.70382	0.31291E-02	0.26430	0.12086E-01	16.370	
2	0.70411	0.31196E-02	0.26399	0.12100E-01	16.671	
7	0.71809	0.28886E-02	0.26248	0.12446E-01	24.278	
8	0.73047	0.28633E-02	0.26066	0.12484E-01	29.213	
9	0.73427	0.27997E-02	0.26005	0.12582E-01	30.511	
10	0.74474	0.26421E-02	0.25828	0.12826E-01	33.693	
13	0.87288	0.16465E-02	0.21285	0.13846E-01	51.600	
14	0.88039		0.20506		51.675	

STAGE	MARANGONI INDEX	FLOW PARAM	QR	REDUCED F-FACTOR
	DYNE/CM		L/MIN	(GM-L) **.5/MIN
1		0.66677E-01	4288.5	0.11352E+06
2	0.30082	0.50749E-01	4278.6	0.11328E+06
7	3.1253	0.46790E-01	3987.3	0.10663E+06
8	-4.1150	0.71301E-01	4429.5	0.11948E+06
9	1.2983	0.70565E-01	4344.7	0.11751E+06
10	3.1816	0.68683E-01	4139.9	0.11278E+06
13	2.4104	0.54282E-01	2966.5	87560.
14	0.74934E-01		0.0000	0.0000

 ***** TRAY SIZING CALCULATIONS *****

 *** SECTION 1 ***

STARTING STAGE NUMBER 2
 ENDING STAGE NUMBER 13
 FLOODING CALCULATION METHOD GLITSCH6

DESIGN PARAMETERS

```

-----
PEAK CAPACITY FACTOR                1.00000
SYSTEM FOAMING FACTOR                1.00000
FLOODING FACTOR                      0.80000
MINIMUM COLUMN DIAMETER              METER 0.30480
MINIMUM DC AREA/COLUMN AREA          0.100000
HOLE AREA/ACTIVE AREA                0.100000
DOWNCOMER DESIGN BASIS                EQUAL FLOW PATH LENGTH

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ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE 12

U-O-S BLOCK SECTION

BLOCK: NRTLDIST MODEL: RADFRAC (CONTINUED)

TRAY SPECIFICATIONS

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TRAY TYPE                            SIEVE
NUMBER OF PASSES                      2
TRAY SPACING                          METER 0.60960

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***** SIZING RESULTS @ STAGE WITH MAXIMUM DIAMETER *****

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STAGE WITH MAXIMUM DIAMETER          8
COLUMN DIAMETER                      METER 1.04798
DC AREA/COLUMN AREA                  0.087500
SIDE DOWNCOMER VELOCITY              M/SEC 0.069606
FLOW PATH LENGTH PER PANEL           METER 0.38082
SIDE DOWNCOMER WIDTH                 METER 0.10198
SIDE WEIR LENGTH                     METER 0.62119
CENTER DOWNCOMER WIDTH               METER 0.082393
CENTER WEIR LENGTH                   METER 1.04474
OFF-CENTER DOWNCOMER WIDTH           METER 0.0
OFF-CENTER SHORT WEIR LENGTH          METER MISSING
OFF-CENTER LONG WEIR LENGTH           METER MISSING
TRAY CENTER TO OCDC CENTER           METER 0.0

```

**** SIZING PROFILES ****

STAGE	DIAMETER	TOTAL AREA	ACTIVE AREA	SIDE DC AREA
	METER	SQM	PER PANEL	PER PANEL
			SQM	SQM
2	1.0480	0.86257	0.34503	0.37738E-01
3	1.0480	0.86257	0.34503	0.37738E-01
4	1.0480	0.86257	0.34503	0.37738E-01
5	1.0480	0.86257	0.34503	0.37738E-01
6	1.0480	0.86257	0.34503	0.37738E-01
7	1.0480	0.86257	0.34503	0.37738E-01
8	1.0480	0.86257	0.34503	0.37738E-01
9	1.0480	0.86257	0.34503	0.37738E-01
10	1.0480	0.86257	0.34503	0.37738E-01
11	1.0480	0.86257	0.34503	0.37738E-01

12	1.0480	0.86257	0.34503	0.37738E-01
13	1.0480	0.86257	0.34503	0.37738E-01

**** ADDITIONAL SIZING PROFILES ****

STAGE	FLOODING FACTOR	PRES. DROP BAR	DC BACKUP METER	DC BACKUP/ (TSPC+WHT)
2	76.52	0.8396E-02	0.2225	33.69
3	76.17	0.8350E-02	0.2213	33.50
4	75.61	0.8279E-02	0.2193	33.21
5	74.73	0.8170E-02	0.2163	32.76
6	73.34	0.8000E-02	0.2117	32.05
7	71.14	0.7743E-02	0.2045	30.97
8	80.00	0.9371E-02	0.2402	36.37
9	78.43	0.9148E-02	0.2343	35.48
10	74.64	0.8639E-02	0.2207	33.42
11	66.42	0.7669E-02	0.1942	29.41
12	56.44	0.6778E-02	0.1676	25.38
13	53.69	0.6588E-02	0.1596	24.17

ASPEN PLUS PLAT: WIN-X64 VER: 37.0

04/15/2021 PAGE 13

U-O-S BLOCK SECTION

BLOCK: NRTLDIST MODEL: RADFRAC (CONTINUED)

STAGE	HEIGHT OVER WEIR METER	DC REL FROTH DENS	TR LIQ REL FROTH DENS	FRA APPR TO SYS LIMIT
2	0.3607E-01	0.6055	0.1780	55.28
3	0.3580E-01	0.6056	0.1783	54.64
4	0.3537E-01	0.6056	0.1788	53.66
5	0.3470E-01	0.6057	0.1795	52.19
6	0.3363E-01	0.6058	0.1808	50.04
7	0.3193E-01	0.6060	0.1829	46.99
8	0.4738E-01	0.6064	0.1743	50.13
9	0.4622E-01	0.6065	0.1754	48.66
10	0.4338E-01	0.6067	0.1783	45.31
11	0.3718E-01	0.6073	0.1862	38.79
12	0.2964E-01	0.6079	0.1988	31.99
13	0.2687E-01	0.6081	0.2035	29.98

BLOCK: PUMP MODEL: PUMP

 INLET STREAM: LIQOVHD
 OUTLET STREAM: S-13
 PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS
 HENRY-COMPS ID: HC-1

*** MASS AND ENERGY BALANCE ***
 IN OUT

TOTAL BALANCE

RELATIVE DIFF.

MOLE (KMOL/HR)	182.425	182.425	0.00000
MASS (KG/HR)	4536.17	4536.17	0.00000
ENTHALPY (CAL/SEC)	-0.320171E+07	-0.320116E+07	-0.170526E-03

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	0.00000	KG/HR
PRODUCT STREAMS CO2E	0.00000	KG/HR
NET STREAMS CO2E PRODUCTION	0.00000	KG/HR
UTILITIES CO2E PRODUCTION	0.00000	KG/HR
TOTAL CO2E PRODUCTION	0.00000	KG/HR

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE 14

U-O-S BLOCK SECTION

BLOCK: PUMP MODEL: PUMP (CONTINUED)

*** INPUT DATA ***

PRESSURE CHANGE BAR	5.00000
DRIVER EFFICIENCY	1.00000

FLASH SPECIFICATIONS:

2 PHASE FLASH	
MAXIMUM NUMBER OF ITERATIONS	30
TOLERANCE	0.000100000

*** RESULTS ***

VOLUMETRIC FLOW RATE L/MIN	87.9419
PRESSURE CHANGE BAR	5.00000
NPSH AVAILABLE M-KGF/KG	-0.033589
FLUID POWER KW	0.73285
BRAKE POWER KW	2.28589
ELECTRICITY KW	2.28589
PUMP EFFICIENCY USED	0.32060
NET WORK REQUIRED KW	2.28589
HEAD DEVELOPED M-KGF/KG	59.3071

NEGATIVE NPSH MAY BE DUE TO VAPOR IN THE FEED OR UNACCOUNTED SUCTION HEAD.

BLOCK: RADFRAC MODEL: RADFRAC

 INLETS - FLASHLIQ STAGE 8
 OUTLETS - VAPOVHD STAGE 1
 LIQOVHD STAGE 1
 BTM STAGE 12

PROPERTY OPTION SET: NRTL RENON (NRTL) / IDEAL GAS

*** MASS AND ENERGY BALANCE ***

	IN	OUT	RELATIVE DIFF.
TOTAL BALANCE			
MOLE (KMOL/HR)	532.342	532.342	0.00000
MASS (KG/HR)	78799.3	78799.3	-0.345503E-07
ENTHALPY (CAL/SEC)	-0.152571E+08	-0.144530E+08	-0.527041E-01

*** CO2 EQUIVALENT SUMMARY ***

FEED STREAMS CO2E	0.00000	KG/HR
PRODUCT STREAMS CO2E	0.00000	KG/HR
NET STREAMS CO2E PRODUCTION	0.00000	KG/HR
UTILITIES CO2E PRODUCTION	0.00000	KG/HR
TOTAL CO2E PRODUCTION	0.00000	KG/HR

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE 15

U-O-S BLOCK SECTION

BLOCK: RADFRAC MODEL: RADFRAC (CONTINUED)

 **** INPUT DATA ****

**** INPUT PARAMETERS ****

NUMBER OF STAGES	12
ALGORITHM OPTION	STANDARD
ABSORBER OPTION	NO
INITIALIZATION OPTION	STANDARD
HYDRAULIC PARAMETER CALCULATIONS	NO
INSIDE LOOP CONVERGENCE METHOD	BROYDEN
DESIGN SPECIFICATION METHOD	NESTED
MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS	100
MAXIMUM NO. OF INSIDE LOOP ITERATIONS	10
MAXIMUM NUMBER OF FLASH ITERATIONS	30
FLASH TOLERANCE	0.000100000
OUTSIDE LOOP CONVERGENCE TOLERANCE	0.000100000

**** COL-SPECS ****

MASS VAPOR DIST / TOTAL DIST	0.018000
MASS REFLUX RATIO	3.00000
MASS BOTTOMS RATE	74,180.0

**** PROFILES ****

P-SPEC	STAGE	1	PRES, BAR	0.066661
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 **** RESULTS ****

*** COMPONENT SPLIT FRACTIONS ***

COMPONENT:	OUTLET STREAMS		
	-----	-----	-----
	VAPOVHD	LIQOVHD	BTM
WATER	.43595E-02	.99454	.11008E-02
METHANOL	.25109E-01	.97489	.11651E-06
H2	.99975	.24810E-03	0.0000

1-DOD-01 0.0000 0.0000 1.0000

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE 16

U-O-S BLOCK SECTION

BLOCK: RADFRAC MODEL: RADFRAC (CONTINUED)

*** SUMMARY OF KEY RESULTS ***

TOP STAGE TEMPERATURE	C	10.2489
BOTTOM STAGE TEMPERATURE	C	189.321
TOP STAGE LIQUID FLOW	KMOL/HR	557.306
BOTTOM STAGE LIQUID FLOW	KMOL/HR	346.097
TOP STAGE VAPOR FLOW	KMOL/HR	3.82014
BOILUP VAPOR FLOW	KMOL/HR	359.932
MOLAR REFLUX RATIO		2.99233
MOLAR BOILUP RATIO		1.03997
CONDENSER DUTY (W/O SUBCOOL)	CAL/SEC	-2,103,790.
REBOILER DUTY	CAL/SEC	2,907,900.

**** MAXIMUM FINAL RELATIVE ERRORS ****

DEW POINT	0.12806E-03	STAGE= 11
BUBBLE POINT	0.68941E-04	STAGE= 12
COMPONENT MASS BALANCE	0.53559E-05	STAGE= 8 COMP=H2
ENERGY BALANCE	0.20388E-03	STAGE= 11

**** PROFILES ****

NOTE REPORTED VALUES FOR STAGE LIQUID AND VAPOR RATES ARE THE FLOWS FROM THE STAGE INCLUDING ANY SIDE PRODUCT.

STAGE	TEMPERATURE C	PRESSURE BAR	ENTHALPY CAL/MOL		HEAT DUTY CAL/SEC
			LIQUID	VAPOR	
1	10.249	0.66661E-01	-63183.	-35149.	-.21038+07
2	29.648	0.73327E-01	-67012.	-52853.	
3	36.434	0.74706E-01	-67745.	-55554.	
7	39.079	0.80222E-01	-67829.	-56205.	
8	51.588	0.81601E-01	-98787.	-56094.	
9	53.914	0.82980E-01	-98422.	-57271.	
10	58.643	0.84359E-01	-0.10434E+06	-57456.	
11	139.22	0.85738E-01	-0.12251E+06	-62106.	
12	189.32	0.87117E-01	-0.11664E+06	-99072.	.29079+07

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE 17

U-O-S BLOCK SECTION

BLOCK: RADFRAC MODEL: RADFRAC (CONTINUED)

STAGE	FLOW RATE		FEED RATE			PRODUCT RATE	
	KMOL/HR		KMOL/HR			KMOL/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	739.7	3.820				182.4247	3.8201
2	546.3	743.6					
3	548.2	732.6					
7	542.0	735.4					
8	747.1	728.3	369.6322	162.7096			
9	755.6	401.0					
10	694.8	409.5					
11	706.0	348.7					
12	346.1	359.9				346.0970	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE		FEED RATE			PRODUCT RATE	
	KG/HR		KG/HR			KG/HR	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.1839E+05	83.15				4536.1740	83.1478
2	0.1068E+05	0.1848E+05					
3	0.1010E+05	0.1530E+05					
7	9920.	0.1465E+05					
8	0.8156E+05	0.1454E+05	.74495+05	4304.1033			
9	0.8160E+05	7385.					
10	0.8773E+05	7424.					
11	0.1484E+06	0.1355E+05					
12	0.7418E+05	0.7418E+05				.74180+05	

STAGE	**** MOLE-X-PROFILE ****			
	WATER	METHANOL	H2	1-DOD-01
1	0.51160	0.48840	0.15186E-05	0.23573E-28
2	0.89016	0.10984	0.81703E-08	0.88271E-24
3	0.97028	0.29719E-01	0.80709E-08	0.11437E-19
7	0.98159	0.18260E-01	0.85645E-08	0.15366E-03
8	0.52254	0.14278E-01	0.87159E-08	0.46318
9	0.53948	0.24684E-02	0.93489E-13	0.45805
10	0.44834	0.37244E-03	0.10087E-17	0.55128
11	0.21700E-01	0.59120E-05	0.11943E-22	0.97829
12	0.29848E-03	0.30766E-07	0.14145E-27	0.99970

STAGE	**** MOLE-Y-PROFILE ****			
	WATER	METHANOL	H2	1-DOD-01
1	0.10709	0.60069	0.29222	0.60442E-34
2	0.50952	0.48898	0.15029E-02	0.23452E-28
3	0.79181	0.20667	0.15243E-02	0.65830E-24
7	0.86058	0.13790	0.15183E-02	0.10985E-07
8	0.85927	0.13908	0.15333E-02	0.11436E-03
9	0.97326	0.26601E-01	0.16238E-07	0.13895E-03
10	0.99519	0.45546E-02	0.17250E-12	0.25371E-03
11	0.89308	0.74210E-03	0.20100E-17	0.10618
12	0.42278E-01	0.11567E-04	0.23427E-22	0.95771

U-O-S BLOCK SECTION

BLOCK: RADFRAC MODEL: RADFRAC (CONTINUED)

**** K-VALUES ****				
STAGE	WATER	METHANOL	H2	1-DOD-01
1	0.20932	1.2299	0.19243E+06	0.25640E-05
2	0.57239	4.4518	0.18394E+06	0.26568E-04
3	0.81606	6.9540	0.18886E+06	0.57558E-04
7	0.87672	7.5522	0.17728E+06	0.71492E-04
8	1.6444	9.7408	0.17591E+06	0.24691E-03
9	1.8040	10.776	0.17368E+06	0.30337E-03
10	2.2197	12.228	0.17098E+06	0.46028E-03
11	41.154	125.51	0.16825E+06	0.10855
12	141.64	375.94	0.16559E+06	0.95807

**** MASS-X-PROFILE ****				
STAGE	WATER	METHANOL	H2	1-DOD-01
1	0.37065	0.62935	0.12311E-06	0.20324E-27
2	0.82003	0.17997	0.84222E-09	0.96772E-23
3	0.94834	0.51664E-01	0.88270E-09	0.13303E-18
7	0.96623	0.31970E-01	0.94336E-09	0.18000E-02
8	0.86228E-01	0.41906E-02	0.16094E-09	0.90958
9	0.89991E-01	0.73235E-03	0.17450E-14	0.90928
10	0.63961E-01	0.94502E-04	0.16103E-19	0.93594
11	0.18604E-02	0.90150E-06	0.11458E-24	0.99814
12	0.25088E-04	0.45995E-08	0.13304E-29	0.99997

**** MASS-Y-PROFILE ****				
STAGE	WATER	METHANOL	H2	1-DOD-01
1	0.88637E-01	0.88430	0.27065E-01	0.59535E-33
2	0.36938	0.63050	0.12192E-03	0.20233E-27
3	0.68285	0.31700	0.14709E-03	0.67561E-23
7	0.77808	0.22177	0.15361E-03	0.11820E-06
8	0.77539	0.22323	0.15482E-03	0.12281E-02
9	0.95210	0.46284E-01	0.17775E-08	0.16177E-02
10	0.98895	0.80501E-02	0.19182E-13	0.30004E-02
11	0.41386	0.61165E-03	0.10423E-18	0.58553
12	0.36958E-02	0.17984E-05	0.22915E-24	0.99630

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE 19

U-O-S BLOCK SECTION

BLOCK: RADFRAC MODEL: RADFRAC (CONTINUED)

 ***** HYDRAULIC PARAMETERS *****

*** DEFINITIONS ***

MARANGONI INDEX = SIGMA - SIGMATO
 FLOW PARAM = (ML/MV)*SQRT(RHOV/RHOL)
 QR = QV*SQRT(RHOV/(RHOL-RHOV))
 F FACTOR = QV*SQRT(RHOV)

WHERE:

SIGMA IS THE SURFACE TENSION OF LIQUID FROM THE STAGE
 SIGMATO IS THE SURFACE TENSION OF LIQUID TO THE STAGE
 ML IS THE MASS FLOW OF LIQUID FROM THE STAGE
 MV IS THE MASS FLOW OF VAPOR TO THE STAGE
 RHOL IS THE MASS DENSITY OF LIQUID FROM THE STAGE
 RHOV IS THE MASS DENSITY OF VAPOR TO THE STAGE
 QV IS THE VOLUMETRIC FLOW RATE OF VAPOR TO THE STAGE

TEMPERATURE

STAGE	C	
	LIQUID FROM	VAPOR TO
1	10.249	29.648
2	29.648	36.434
3	36.434	37.929
7	39.079	51.588
8	51.588	66.605
9	53.914	58.643
10	58.643	139.22
11	139.22	189.32
12	189.32	189.32

STAGE	MASS FLOW KG/HR		VOLUME FLOW L/MIN		MOLECULAR WEIGHT	
	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO
1	18394.	18477.	353.71	0.42547E+07	24.866	24.850
2	10684.	15303.	188.90	0.42066E+07	19.556	20.890
3	10104.	14723.	173.81	0.41608E+07	18.432	20.048
7	9919.6	14539.	170.27	0.40160E+07	18.302	19.964
8	81565.	11689.	1379.2	0.32525E+07	109.17	20.735
9	81603.	7423.7	1385.1	0.22318E+07	108.00	18.129
10	87734.	13555.	1455.7	0.23238E+07	126.28	38.876
11	0.14836E+06	74177.	2359.8	0.26478E+07	210.13	206.09
12	74180.	0.0000	1250.1	0.0000	214.33	

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE 20

U-O-S BLOCK SECTION

BLOCK: RADFRAC MODEL: RADFRAC (CONTINUED)

STAGE	DENSITY GM/CC		VISCOSITY CP		SURFACE TENSION DYNE/CM
	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM
1	0.86672	0.72379E-04	0.93262	0.10131E-01	50.086
2	0.94261	0.60630E-04	0.78257	0.10374E-01	66.286
3	0.96885	0.58975E-04	0.70992	0.10400E-01	68.990

7	0.97099	0.60337E-04	0.67844	0.10903E-01	69.040
8	0.98564	0.59898E-04	5.0823	0.11472E-01	47.883
9	0.98192	0.55438E-04	4.6475	0.11036E-01	48.332
10	1.0045	0.97217E-04	6.2589	0.12953E-01	44.032
11	1.0478	0.46692E-03	3.1258	0.76923E-02	20.562
12	0.98896		1.0211		16.087

STAGE	MARANGONI INDEX DYNE/CM	FLOW PARAM	QR L/MIN	REDUCED F-FACTOR (GM-L) **.5/MIN
1		0.90972E-02	38883.	0.11447E+07
2	16.200	0.55991E-02	33739.	0.10358E+07
3	2.7040	0.53541E-02	32463.	0.10104E+07
7	-.69067E-01	0.53783E-02	31659.	0.98648E+06
8	1.0464	0.54396E-01	25356.	0.79602E+06
9	0.44896	0.82595E-01	16770.	0.52549E+06
10	-4.2994	0.63677E-01	22862.	0.72455E+06
11	-23.470	0.42220E-01	55906.	0.18093E+07
12	-4.4752		0.0000	0.0000

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE 21

U-O-S BLOCK SECTION

BLOCK: RADFRAC MODEL: RADFRAC (CONTINUED)

 ***** TRAY SIZING CALCULATIONS *****

 *** SECTION 1 ***

STARTING STAGE NUMBER	2
ENDING STAGE NUMBER	11
FLOODING CALCULATION METHOD	GLITSCH6

DESIGN PARAMETERS

PEAK CAPACITY FACTOR	1.00000	
SYSTEM FOAMING FACTOR	1.00000	
FLOODING FACTOR	0.80000	
MINIMUM COLUMN DIAMETER	METER	0.30480
MINIMUM DC AREA/COLUMN AREA	0.100000	
HOLE AREA/ACTIVE AREA	0.100000	
DOWNCOMER DESIGN BASIS	EQUAL FLOW PATH LENGTH	

TRAY SPECIFICATIONS

TRAY TYPE	SIEVE
NUMBER OF PASSES	2

TRAY SPACING METER 0.60960

***** SIZING RESULTS @ STAGE WITH MAXIMUM DIAMETER *****

STAGE WITH MAXIMUM DIAMETER		11
COLUMN DIAMETER	METER	4.26049
DC AREA/COLUMN AREA		0.087500
SIDE DOWNCOMER VELOCITY	M/SEC	0.031529
FLOW PATH LENGTH PER PANEL	METER	1.54818
SIDE DOWNCOMER WIDTH	METER	0.41458
SIDE WEIR LENGTH	METER	2.52542
CENTER DOWNCOMER WIDTH	METER	0.33496
CENTER WEIR LENGTH	METER	4.24730
OFF-CENTER DOWNCOMER WIDTH	METER	0.0
OFF-CENTER SHORT WEIR LENGTH	METER	MISSING
OFF-CENTER LONG WEIR LENGTH	METER	MISSING
TRAY CENTER TO OCDC CENTER	METER	0.0

**** SIZING PROFILES ****

STAGE	DIAMETER	TOTAL AREA	ACTIVE AREA	SIDE DC AREA
	METER	SQM	PER PANEL SQM	PER PANEL SQM
2	4.2605	14.256	5.7025	0.62372
3	4.2605	14.256	5.7025	0.62372
4	4.2605	14.256	5.7025	0.62372
5	4.2605	14.256	5.7025	0.62372
6	4.2605	14.256	5.7025	0.62372
7	4.2605	14.256	5.7025	0.62372
8	4.2605	14.256	5.7025	0.62372
9	4.2605	14.256	5.7025	0.62372
10	4.2605	14.256	5.7025	0.62372

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE 22

U-O-S BLOCK SECTION

BLOCK: RADFRAC MODEL: RADFRAC (CONTINUED)

STAGE	DIAMETER	TOTAL AREA	ACTIVE AREA	SIDE DC AREA
	METER	SQM	PER PANEL SQM	PER PANEL SQM
11	4.2605	14.256	5.7025	0.62372

**** ADDITIONAL SIZING PROFILES ****

STAGE	FLOODING FACTOR	PRES. DROP BAR	DC BACKUP METER	DC BACKUP/ (TSPC+WHT)
2	63.04	0.5108E-02	0.1317	19.95
3	60.91	0.5146E-02	0.1308	19.80

4	60.10	0.5134E-02	0.1306	19.77
5	59.45	0.5115E-02	0.1305	19.76
6	58.83	0.5096E-02	0.1304	19.75
7	59.18	0.5096E-02	0.1304	19.74
8	52.29	0.5334E-02	0.1526	23.11
9	36.90	0.5249E-02	0.1623	24.57
10	44.26	0.5368E-02	0.1551	23.49
11	80.00	0.9333E-02	0.1957	29.63

STAGE	HEIGHT OVER WEIR METER	DC REL FROTH DENS	TR LIQ REL FROTH DENS	FRA APPR TO SYS LIMIT
2	0.9913E-02	0.6082	0.2559	19.24
3	0.9264E-02	0.6082	0.2605	18.45
4	0.9160E-02	0.6083	0.2624	18.24
5	0.9119E-02	0.6083	0.2640	18.09
6	0.9086E-02	0.6083	0.2656	17.95
7	0.9031E-02	0.6083	0.2652	18.00
8	0.3296E-01	0.6083	0.3099	15.87
9	0.2754E-01	0.6083	0.4069	10.46
10	0.3269E-01	0.6083	0.3311	14.71
11	0.6796E-01	0.6083	0.1807	44.37

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE 23

STREAM SECTION

BTM FEED FLASHLIQ FLASHVAP LIQOVHD

STREAM ID	BTM	FEED	FLASHLIQ	FLASHVAP	LIQOVHD
FROM :	RADFRAC	----	FLASH	FLASH	RADFRAC
TO :	----	FLASH	RADFRAC	----	PUMP
SUBSTREAM: MIXED					
PHASE:	LIQUID	MIXED	LIQUID	VAPOR	LIQUID
COMPONENTS: KMOL/HR					
WATER	0.1033	95.0000	93.8404	1.1596	93.3280
METHANOL	1.0648-05	95.0000	91.3912	3.6088	89.0965
H2	4.8955-26	71.0000	1.1166	69.8834	2.7703-04
1-DOD-01	345.9937	346.0000	345.9937	6.3216-03	4.3003-27
TOTAL FLOW:					
KMOL/HR	346.0970	607.0000	532.3419	74.6581	182.4247
KG/HR	7.4180+04	7.9078+04	7.8799+04	278.7560	4536.1740
L/MIN	1250.1382	2982.1838	1356.9809	1649.6454	87.2283
STATE VARIABLES:					
TEMP C	189.3206	120.0000	119.9899	119.9899	10.2489
PRES BAR	8.7117-02	25.0000	24.6553	24.6553	6.6661-02
VFRAC	0.0	0.1229	0.0	1.0000	0.0
LFRAC	1.0000	0.8771	1.0000	0.0	1.0000
SFRAC	0.0	0.0	0.0	0.0	0.0
ENTHALPY:					
CAL/MOL	-1.1664+05	-9.0800+04	-1.0318+05	-2546.0687	-6.3183+04
CAL/GM	-544.2225	-696.9788	-697.0322	-681.9035	-2540.9428

CAL/SEC	-1.1214+07	-1.5310+07	-1.5257+07	-5.2801+04	-3.2017+06
ENTROPY:					
CAL/MOL-K	-324.0686	-209.6870	-238.3190	-5.5024	-48.3310
CAL/GM-K	-1.5120	-1.6095	-1.6100	-1.4737	-1.9437
DENSITY:					
MOL/CC	4.6141-03	3.3924-03	6.5383-03	7.5428-04	3.4856-02
GM/CC	0.9890	0.4419	0.9678	2.8163-03	0.8667
AVG MW	214.3330	130.2769	148.0239	3.7338	24.8660

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE 24

STREAM SECTION

METHANOL S-13 VAPOVHD WATER

STREAM ID	METHANOL	S-13	VAPOVHD	WATER
FROM :	NRTLDIST	PUMP	RADFRAC	NRTLDIST
TO :	----	NRTLDIST	----	----
SUBSTREAM: MIXED				
PHASE:	LIQUID	LIQUID	VAPOR	LIQUID
COMPONENTS: KMOL/HR				
WATER	0.6333	93.3280	0.4091	92.6946
METHANOL	88.6509	89.0965	2.2947	0.4455
H2	2.7703-04	2.7703-04	1.1163	9.4332-31
1-DOD-01	0.0	4.3003-27	2.3090-34	0.0
TOTAL FLOW:				
KMOL/HR	89.2845	182.4247	3.8201	93.1402
KG/HR	2851.9777	4536.1740	83.1478	1684.1963
L/MIN	67.5353	87.2888	2.2505+04	31.8834
STATE VARIABLES:				
TEMP C	94.9288	10.8053	10.2489	132.5312
PRES BAR	3.0000	5.0667	6.6661-02	3.0000
VFRAC	0.0	0.0	1.0000	0.0
LFRAC	1.0000	1.0000	0.0	1.0000
SFRAC	0.0	0.0	0.0	0.0
ENTHALPY:				
CAL/MOL	-5.5209+04	-6.3172+04	-3.5149+04	-6.6158+04
CAL/GM	-1728.3733	-2540.5095	-1614.8730	-3658.6902
CAL/SEC	-1.3692+06	-3.2012+06	-3.7298+04	-1.7117+06
ENTROPY:				
CAL/MOL-K	-52.0430	-48.2941	-12.9817	-33.2369
CAL/GM-K	-1.6293	-1.9422	-0.5964	-1.8381
DENSITY:				
MOL/CC	2.2034-02	3.4832-02	2.8291-06	4.8688-02
GM/CC	0.7038	0.8661	6.1577-05	0.8804
AVG MW	31.9426	24.8660	21.7656	18.0824

ASPEN PLUS PLAT: WIN-X64 VER: 37.0 04/15/2021 PAGE 25

PROBLEM STATUS SECTION

BLOCK STATUS

```
*****  
*                                                                 *  
* Calculations were completed normally                          *  
*                                                                 *  
* All Unit Operation blocks were completed normally            *  
*                                                                 *  
* All streams were flashed normally                             *  
*                                                                 *  
*****
```

BOL Refining Calculations

Flash Column (T-101)

The sizing of the flash column was done empirically using the equations shown below.

$$F_{LV} = \frac{W_L}{W_V} \sqrt{\frac{\rho_V}{\rho_L}}$$

Where W_L and W_V are the mass flow rates of the liquid and the vapor products respectively, and ρ_V and ρ_L are the densities of the vapor and the liquid products respectively.

$$K_d = e^{A+B \ln F_{LV} + C(\ln F_{LV})^2 + D(\ln F_{LV})^3 + E(\ln F_{LV})^4}$$

$$A = -1.877478$$

$$B = -0.814580$$

$$C = -0.187074$$

$$D = -0.014523$$

$$E = -0.001015$$

K_d is the K value of the drum and it is an empirical constant based off of experimental data.

$$u_{perm} = K_d \sqrt{\frac{\rho_L - \rho_V}{\rho_V}}$$

Where u_{perm} is the permissible vapor velocity, K_d is the drum constant, and ρ_V and ρ_L are the vapor and liquid densities respectively.

$$A_c = \frac{V \times MW_V}{u_{perm} \times \rho_V}$$

The cross-sectional area of the flash drum, A_c , can then be calculated where V is the molar flow rate of the vapor, MW_V is the molecular mass of the vapor, u_{perm} is the permissible vapor velocity, and ρ_V is the density of the vapor.

$$D = \sqrt{\frac{4A_c}{\pi}}$$

Knowing the cross-sectional area of the column will allow the diameter of the column to be determined. For vertical vessels, it is common to keep the height to diameter (L/D) ratio between 3 and 5. For this process, the assumed L/D ratio was 4.

$$L = 4D$$

Distillation Columns (T-102 and T-103)

Tray Efficiency and Number of Actual Trays

The distillation column was modeled in Aspen using RADFRAC to allow for interactive column sizing. RADFRAC reports theoretical number of trays, so tray efficiency for the distillation column was assumed to be 50%.

$$E_o = \frac{\textit{number of theoretical trays}}{\textit{number of actual trays}}$$

where E_o = tray efficiency

For distillation column 1 (T-102):

$$0.50 = \frac{12}{\textit{number of actual trays}}$$

$$\textit{number of actual trays} = \frac{12}{0.50} = 24$$

Column Height

To calculate the height of the distillation columns, an additional 15% of height based on the number of trays and the tray spacing was added to provide for extra space at the top and bottom of the column. This extra height allows for disengaging space at the top of the column and allows for a small liquid reservoir to form at the bottom of the column.

$$H_T = N_T \times \textit{tray spacing}$$

Where N_T is the number of trays and H_T is the height based only on the number of trays and the tray spacing.

$$H_A = H_T + 0.15H_T$$

Where H_T is the height of the column based on number of trays and tray spacing, and H_A is the actual height of the column with the additional 15% of space included.

Reflux Drum Sizing (V-100 & V-101)

Modeled after standard, horizontally positioned reflux drums, the reflux drums for this process were designed to contain 5 minutes of liquid holdup with the drum half full and an assumed length to diameter ratio of 3.

$$V = \dot{v} \times 2 \times 5min$$

Where \dot{v} is the volumetric flow rate of the liquid from the top stage of the column.

$$V = \frac{\pi}{4} D^2 L$$

Using the first equation to determine the volume of the fluid in the drum, the length and diameter of the drum can be found using the equation for the volume of a cylinder, with an assumed L/D ratio of 3.

Heat Exchanger Sizing (E-107, E-108, E-109, and E-110)

The q for the sizing of the heat exchanger was determined by Aspen as the required condenser/reboiler heat duty detailed in the Aspen report.

$$q = UA\Delta T_{lm}$$

Where q is the required heat duty, U is the overall heat transfer coefficient, A is the surface area of the heat exchanger, and ΔT_{lm} is the log mean temperature difference based on a counter flow exchanger.

$$\Delta T_{lm} = \frac{(T_{h,i} - T_{c,o}) - (T_{h,o} - T_{c,i})}{\ln \left(\frac{T_{h,i} - T_{c,o}}{T_{h,o} - T_{c,i}} \right)}$$

Cooling and heating utility incoming temperatures were estimated from Table 27.1 below and found in *Product and Process Design Principles* by Sieder et al., and U values were estimated based off of Table 27.2 shown below.

Table 27.1 Heating and Cooling Utilities – Identifiers and Temperatures Ranges

Identifier	Utility	Typical Operating Range
Hot Utilities—In increasing Cost per BTU:		
<i>lps</i>	Low-pressure steam, 15 to 30 psig	250 to 275°F
<i>mps</i>	Medium-pressure steam, 100 to 150 psig	325 to 366°F
<i>hps</i>	High-pressure steam, 400 to 600 psig	448 to 488°F
<i>fo</i>	Fuel oils	
<i>fg</i>	Fuel gas	Process waste stream
<i>po</i>	Petroleum oils	Below 600°F
<i>dt</i>	Dowtherms	Below 750°F
Cold Utilities—In increasing Cost per BTU:		
<i>bfiw</i>	Boiler feed water	Used to raise process steam
<i>ac</i>	Air cooling	Supply at 85 to 95°F—temperature approach to process 4°F
<i>rw</i>	River water	Supply at 80 to 90°F (from cooling tower), return at 110°F
<i>cw</i>	Cooling water	Supply at 80 to 90°F (from cooling tower), return at 115 to 125°F
<i>cw</i>	Chilled water	45 to 90°F
<i>rb</i>	Refrigerated brine	0 to 50°F
<i>pr</i>	Propane refrigerant	–40 to 20°F

Table 27.2 Typical Overall Heat-Transfer Coefficients for Shell-and-Tube Heat Exchangers
 [U = BTU/(°F-ft²-hr)]

Shell Side	Tube Side	Design U	Includes Total Dirt
<i>Liquid-Liquid Media</i>			
Aroclor 1248	Jet fuels	100–150	0.0015
Cutback asphalt	Water	10–20	0.01
Demineralized water	Water	300–500	0.001
Ethanol amine (MEA or DEA) 10–25% solutions	Water or DEA, or MEA solutions	140–200	0.003
Fuel oil	Water	15–25	0.007
Fuel oil	Oil	10–15	0.008
Gasoline	Water	60–100	0.003
Heavy oils	Heavy oils	10–40	0.004
Heavy oils	Water	15–50	0.005
Hydrogen-rich reformer stream	Hydrogen-rich reformer stream	90–120	0.002
Kerosene or gas oil	Water	25–50	0.005
Kerosene or gas oil	Oil	20–35	0.005
Kerosene or jet fuels	Trichloroethylene	40–50	0.0015
Jacket water	Water	230–300	0.002
Lube oil (low viscosity)	Water	25–50	0.002
Lube oil (high viscosity)	Water	40–80	0.003
Lube oil	Oil	11–20	0.006
Naphtha	Water	50–70	0.005
Naphtha	Oil	25–35	0.005
Organic solvents	Water	50–150	0.003
Organic solvents	Brine	35–90	0.003
Organic solvents	Organic solvents	20–60	0.002
Tall oil derivatives, vegetable oil, etc.	Water	20–50	0.004
Water	Caustic soda solutions (10–30%)	100–250	0.003
Water	Water	200–250	0.003
Wax distillate	Water	15–25	0.005
Wax distillate	Oil	13–23	0.005
<i>Condensing Vapor-liquid Media</i>			
Alcohol vapor	Water	100–200	0.002
Asphalt 450°F	Dowtherm vapor	40–60	0.006
Dowtherm vapor	Tall oil and derivatives	60–80	0.004
Dowtherm vapor	Dowtherm liquid	80–120	0.0015
Gas-plant tar	Steam	40–50	0.0055
High-boiling hydrocarbons V	Water	20–50	0.003
Low-boiling hydrocarbons A	Water	80–200	0.003
Hydrocarbon vapors (partial condenser)	Oil	25–45	0.004
Organic solvents A	Water	100–200	0.003
Organic solvents high NC, A	Water or brine	20–60	0.003
Organic solvents low NC, V	Water or brine	50–120	0.003
Kerosene	Water	30–65	0.004
Kerosene	Oil	20–30	0.005
Naphtha	Water	50–75	0.005
Naphtha	Oil	20–30	0.005
Stabilizer column vapor	Water	80–120	0.003
Steam	Feed water	400–1,000	0.0005
Steam	No. 6 fuel oil	15–25	0.0055
Steam	No. 2 fuel oil	60–90	0.0025
Sulfur dioxide	Water	150–200	0.003
Tall oil derivatives, vegetable oils (vapor)	Water	20–50	0.004
Water	Aromatic vapor-stream azeotrope	40–80	0.005

Table 27.2 (Continued)

Shell Side	Tube Side	Design <i>U</i>	Includes Total Dirt
<i>Gas-liquid Media</i>			
Air, N ₂ , etc. (compressed)	Water or brine	40–80	0.005
Air, N ₂ , etc. A	Water or brine	10–50	0.005
Water or brine	Air, N ₂ , etc. (compressed)	20–40	0.005
Water or brine	Air, N ₂ , etc. A	5–20	0.005
Water	Hydrogen containing natural-gas mixtures	80–125	0.003
<i>Vaporizers</i>			
Anhydrous ammonia	Steam condensing	150–300	0.0015
Chlorine	Steam condensing	150–300	0.0015
Chlorine	Light heat-transfer oil	40–60	0.0015
Propane, butane, etc.	Steam condensing	200–300	0.0015
Water	Steam condensing	250–400	0.0015

NC = Noncondensable gas present

V = Vacuum

A = Atmospheric pressure

Dirt (or fouling factor) units are (hr-ft²-°F/Btu).

To convert British thermal units per hour-square foot-degrees Fahrenheit to joules per square meter-second-Kelvin, multiply by 5.6783; to convert from hr-ft²-°F/Btu to sec-m²-K/joule, multiply by 0.1761.

$$N_{CO_2} = k'_g * A_{int} * (p_{CO_2} - p_{CO_2}^*)_{lm}$$

$$(p_{CO_2} - p_{CO_2}^*)_{lm} = \frac{(p_{CO_2\,bottom} - p_{CO_2\,bottom}^*) - (p_{CO_2\,top} - p_{CO_2\,top}^*)}{\ln \left(\frac{(p_{CO_2\,bottom} - p_{CO_2\,bottom}^*)}{(p_{CO_2\,top} - p_{CO_2\,top}^*)} \right)}$$

Figure 27.1: Absorber Sizing Formulas

Table 27.3 Absorber Sizing Variables

Symbol	Explanation	Units
$p_{CO_2_{bottom}}$	Partial Pressure of CO2 in flue gas IN	Pa
$p_{CO_2_{top}}$	Partial Pressure of CO2 in flue gas OUT	Pa
$p_{CO_2_{bottom}}^*$	CO2 equilibrium partial pressure for the BOL OUT (rich-loaded BOL)	Pa
$p_{CO_2_{top}}^*$	CO2 equilibrium partial pressure for the BOL IN (lean-loaded BOL)	Pa
$(p_{CO_2} - p_{CO_2}^*)_{lm}$	log mean CO2 pressure difference	Pa
k'_g	Liquid Film Mass Transfer Coefficient	$\frac{gmol}{s m^2 Pa}$
N_{CO_2}	100 tonne per day, CO2 Absorption Rate	$\frac{gmol}{s}$
A_{int}	Effective Interfacial Surface Area of Packing	m^2

Table 27.4 Absorber Sizing Calculation

<i>Mass Transfer Coefficient Approach (using log mean pressure differential assumption for dilute mixtures)</i>			
Symbol	Meaning	Units	Magnitude
p_CO2_bottom	Partial Pressure of CO2 in flue gas IN	Pa	16,212
p_CO2_top	Partial Pressure of CO2 in flue gas OUT	Pa	1,621
p*_CO2_bottom	CO2 equilibrium partial pressure for the BOL OUT (rich-loaded BOL)	Pa	8,500
p*_CO2_top	CO2 equilibrium partial pressure for the BOL IN (lean-loaded BOL)	Pa	1,500
(p_CO2-p*_CO2)_lm	log mean CO2 pressure difference	Pa	1,828
k_g'	Liquid Film Mass Transfer Coefficient	gmol/s m ² Pa	6.35E-07
N_CO2	100 tonne per day, CO2 Absorption Rate	gmol/s	26
A_int	Effective Interfacial Surface Area of Packing	m ²	22,664
a	Mellapak 250Y Packing Surface Area/Volume	m ² /m ³	250
V	Volume of Absorber	m ³	91
D/H	Ratio of Height and Diameter of Absorber	-	5
D	Diameter of Absorber	m	4.0
H	Height of Absorber	m	20.0

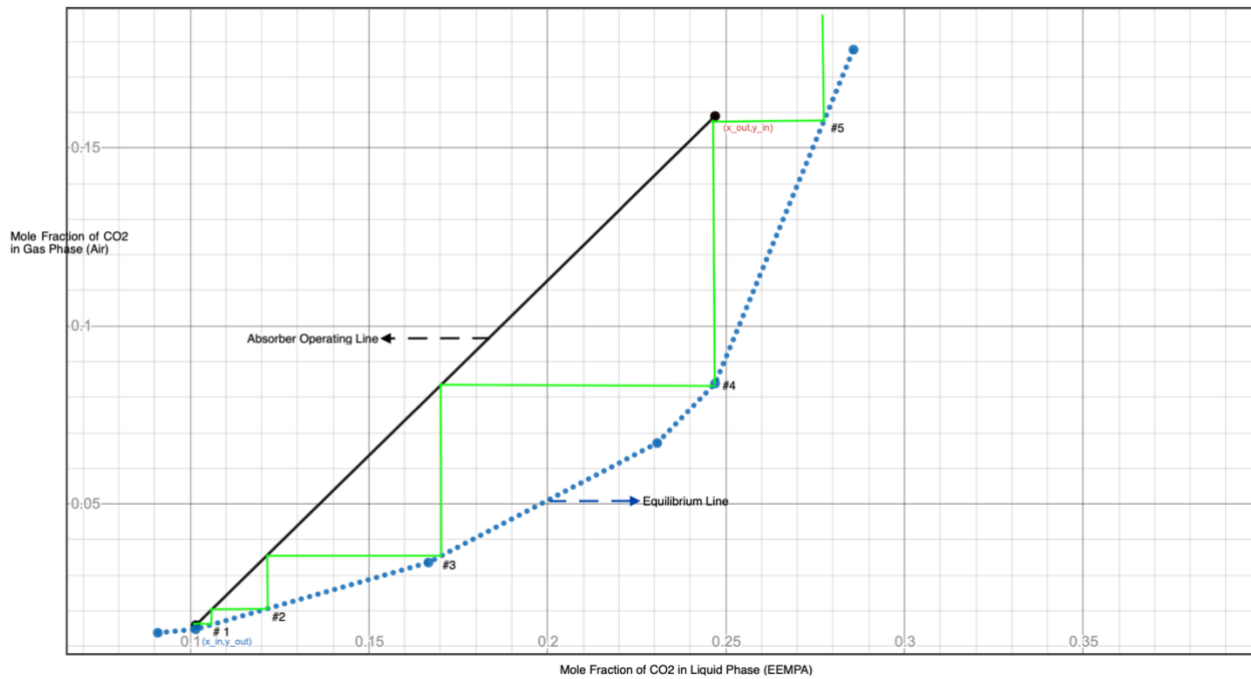


Figure 27.2: McCabe Thiele diagram for absorber to calculate number of theoretical stages

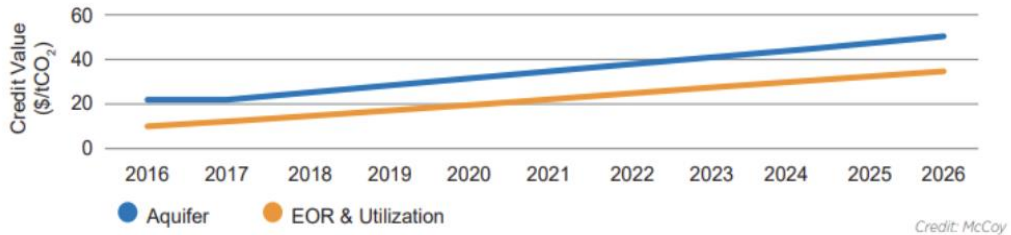
Table 27.5 Reactor Sizing Calculation

Symbol	Description	Units	Value	Source
P	Pressure	bar	25	
T	Temperature	K	398	
m_H2_in	Mole Flow Rate of Hydrogen into the Reactor	mol/s	99	Mass Balance
m_H2_out	Mole Flow Rate of Hydrogen out of the Reactor	mol/s	26	25% Excess
m_H2_cons	Mass Flow Rate of Hydrogen consumed in the Reactor	mol/s	72	Mass Balance
k_L a	volumetric mass transfer coefficient	s ⁻¹	0.12	k_L a bubble column correlations from paper
C_H2_gas	concentration of hydrogen in gas phase	mol/m ³	756	
C_H2_liq	concentration of hydrogen in liquid phase	mol/m ³	-	immediate reaction
V_L	Volume of liquid	m ³	0.8	mass transfer equation
Q	Volumetric Flow Rate of Hydrogen into the Reactor	m ³ /s	0.13	Using Density of Hydrogen
e_G	Gas Holdup		0.20	gas holdup in a bubble column correlations from paper
V_bubble	Volume of hydrogen bubbles	m ³	0.0	
e_G	Gas Holdup		0.20	
V_LG	Volume of Liquid+Gas	m ³	0.8	
V_cat	Volume of Catalyst	m ³	0.5	
V_R	Volume of Reactor	m ³	1.3	
D	reactor diameter	m	0.6	
H	reactor height	m	1.3	Aspect Ratio (H:D) 1.5:1
A	cross-sectional area	m ²	0.33	
u_G	superficial velocity based on total cross-sectional area	ms ⁻¹	0.40	

	Process Variables
	Process Inputs/Outputs
	Calculated Values

45Q, Types of Sources and Credit Between 2018-2026

	Threshold by Facility Type (ktCO ₂ /y0)			Credit in 2026 (\$/t)
	Power Plant	Industrial Facility	Direct Air Capture	
Dedicated Storage	500	100	100	50
EOR	500	100	100	35
Utilization	25	25	25	35



¹ \$35/ton for EOR and \$50/ton for saline storage, available indefinitely

Figure 27.3 Section 45Q Internal Revenue Service

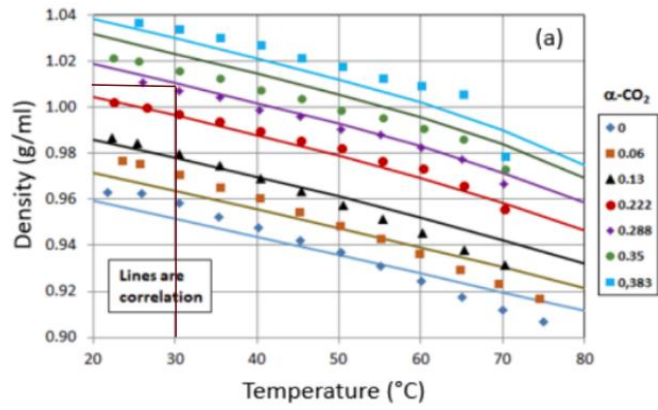


Figure 27.4 The above graph shows variation of density of EEMPA-CO₂-H₂O with temperature

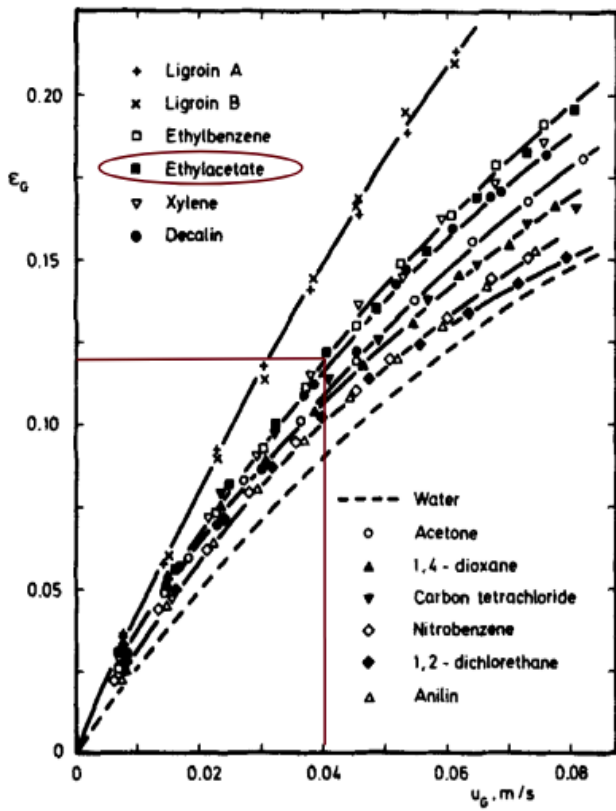


Figure 27.5 Gas holdups in various organic liquids

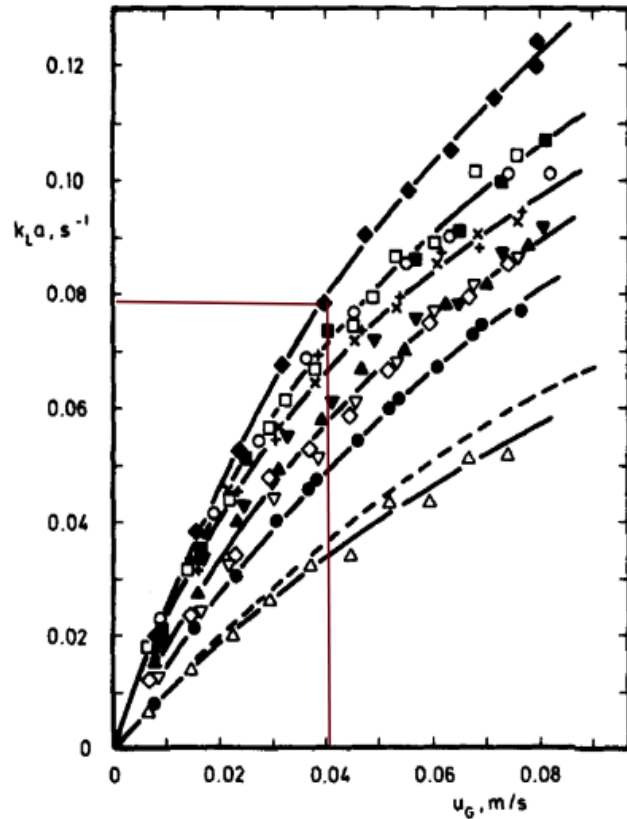


Figure 27.6 Volumetric mass transfer coefficients in various organic liquids. Symbols as in Figure 27.4 to the left.

27. Appendix B: Vendor Specification Sheets

Table 28.1 Physical and Process Parameters for EEMPA

Pure Solvent	Units	Current R&D Value	Target R&D Value	
Molecular Weight	mol ⁻¹	216.3	-	
Normal Boiling Point	°C	181.0	-	
Normal Freezing Point	°C	<0	-	
Vapor Pressure @ 15°C	bar	5E-5	-	
Manufacturing Cost for Solvent	\$/kg	13	10	
Working Solution				
Concentration	kg/kg	0.98 (hydrated)	-	
Specific Gravity (15°C/15°C)	-	0.94	-	
Specific Heat Capacity @ STP	kJ/kg-K	1.95	-	
Viscosity @ 15°C	cP	11.3	-	
Absorption				
Pressure	bar	1	-	
Temperature	°C	40	-	
Equilibrium CO ₂ Loading	mol/mol	0.29	-	
Heat of Absorption	kJ/mol CO ₂	75	-	
Solution Viscosity	cP	25	-	
Desorption				
Pressure	bar	1.8	-	
Temperature	°C	117	-	
Equilibrium CO ₂ Loading	mol/mol	0.05	-	
Heat of Desorption	kJ/mol CO ₂	75	-	

CARBON CAPTURE TECHNOLOGY SHEETS POST-COMBUSTION SOLVENTS

U.S. DEPARTMENT OF ENERGY NATIONAL ENERGY TECHNOLOGY LABORATORY

Proposed Module Design		(for equipment developers)		
Flue Gas Flowrate	kg/hr		2.6E6	
CO ₂ Recovery, Purity, and Pressure	% / % / bar	90	95	150
Absorber Pressure Drop	bar		<0.1	
Estimated Absorber/Stripper Cost of Manufacturing and Installation	$\frac{\$}{\text{kg/hr}}$		pending	

Mellapak 250.Y/X

A highly versatile packing type



0602 2510

Mellapak is the most widely used structured packing worldwide. It has proven excellent performance in columns with diameters up to 15m. It is supplied in sheet metal thicknesses from 0.1 mm up.

Special features

- Pressure drop per theoretical stage 0.3-1.0 mbar
- Pressure drop at 70-80% flooding about 2 mbar/m
- Minimum liquid load approx. $0.2 \text{ m}^3/\text{m}^2\text{h}$
- Maximum liquid load up to more than $200 \text{ m}^3/\text{m}^2\text{h}$ (typically in desorption columns)

Preferred applications

- Vacuum to moderate pressure
- High pressure in selected applications
- Increasing capacity of existing tray and packed columns

Typical applications

- Chemical industry: Ethylbenzene/styrene, tall oil, cyclohexanone/-ol, air separation
- Petrochemical industry: Quench columns, C_3 - and C_4 - splitters, xylene splitters
- Refineries: Vacuum and atmospheric columns
- Absorption: Natural gas drying, CO_2 - and H_2S -absorbers and strippers, ethyleneoxide absorbers and strippers, acrylonitrile absorbers

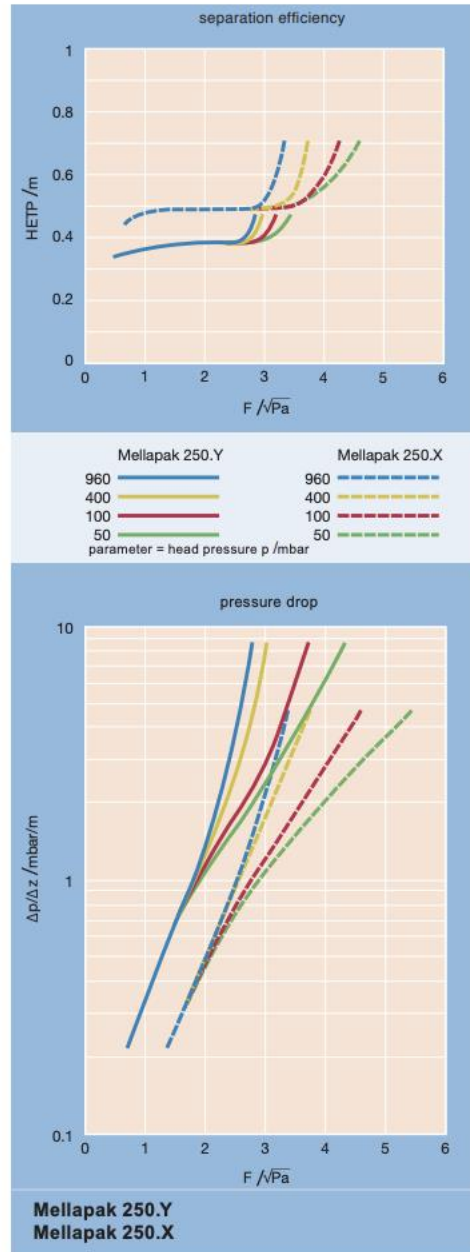


Figure 28.1 The figure summarizes the applications and features of the Sulzer Mellapak 250Y Packing

28. Appendix C: Patents

N/A

30. Appendix D: Material Safety Data Sheets

SAFETY DATA SHEET

Hydrogen

Section 1. Identification

GHS product identifier	: Hydrogen
Chemical name	: hydrogen
Other means of identification	: Dihydrogen; o-Hydrogen; p-Hydrogen; Molecular hydrogen; H ₂ ; UN 1049
Product type	: Gas.
Product use	: Synthetic/Analytical chemistry.
Synonym	: Dihydrogen; o-Hydrogen; p-Hydrogen; Molecular hydrogen; H ₂ ; UN 1049
SDS #	: 001026
Supplier's details	: Airgas USA, LLC and its affiliates 259 North Radnor-Chester Road Suite 100 Radnor, PA 19087-5283 1-610-687-5253
24-hour telephone	: 1-866-734-3438

Section 2. Hazards identification

OSHA/HCS status	: This material is considered hazardous by the OSHA Hazard Communication Standard (29 CFR 1910.1200).
Classification of the substance or mixture	: FLAMMABLE GASES - Category 1 GASES UNDER PRESSURE - Compressed gas

GHS label elements

Hazard pictograms



Signal word

: Danger

Hazard statements

: Extremely flammable gas.
Contains gas under pressure; may explode if heated.
May displace oxygen and cause rapid suffocation.
Burns with invisible flame.
May form explosive mixtures with air.

Precautionary statements

General

: Read and follow all Safety Data Sheets (SDS'S) before use. Read label before use. Keep out of reach of children. If medical advice is needed, have product container or label at hand. Close valve after each use and when empty. Use equipment rated for cylinder pressure. Do not open valve until connected to equipment prepared for use. Use a back flow preventative device in the piping. Use only equipment of compatible materials of construction. Approach suspected leak area with caution.

Prevention

: Keep away from heat, hot surfaces, sparks, open flames and other ignition sources. No smoking.

Response

: Leaking gas fire: Do not extinguish, unless leak can be stopped safely. In case of leakage, eliminate all ignition sources.

Storage

: Protect from sunlight. Store in a well-ventilated place.

Disposal

: Not applicable.

Hazards not otherwise classified

: In addition to any other important health or physical hazards, this product may displace oxygen and cause rapid suffocation.

Section 3. Composition/information on ingredients

Substance/mixture	: Substance
Chemical name	: hydrogen
Other means of identification	: Dihydrogen; o-Hydrogen; p-Hydrogen; Molecular hydrogen; H ₂ ; UN 1049
Product code	: 001026

CAS number/other identifiers

CAS number : 1333-74-0

Ingredient name	%	CAS number
hydrogen	100	1333-74-0

Any concentration shown as a range is to protect confidentiality or is due to batch variation.

There are no additional ingredients present which, within the current knowledge of the supplier and in the concentrations applicable, are classified as hazardous to health or the environment and hence require reporting in this section.

Occupational exposure limits, if available, are listed in Section 8.

Section 4. First aid measures

Description of necessary first aid measures

- Eye contact** : Immediately flush eyes with plenty of water, occasionally lifting the upper and lower eyelids. Check for and remove any contact lenses. Continue to rinse for at least 10 minutes. Get medical attention if irritation occurs.
- Inhalation** : Remove victim to fresh air and keep at rest in a position comfortable for breathing. If not breathing, if breathing is irregular or if respiratory arrest occurs, provide artificial respiration or oxygen by trained personnel. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation. Get medical attention if adverse health effects persist or are severe. If unconscious, place in recovery position and get medical attention immediately. Maintain an open airway. Loosen tight clothing such as a collar, tie, belt or waistband.
- Skin contact** : Flush contaminated skin with plenty of water. Remove contaminated clothing and shoes. To avoid the risk of static discharges and gas ignition, soak contaminated clothing thoroughly with water before removing it. Get medical attention if symptoms occur. Wash clothing before reuse. Clean shoes thoroughly before reuse.
- Ingestion** : As this product is a gas, refer to the inhalation section.

Most important symptoms/effects, acute and delayed

Potential acute health effects

- Eye contact** : Contact with rapidly expanding gas may cause burns or frostbite.
- Inhalation** : No known significant effects or critical hazards.
- Skin contact** : Contact with rapidly expanding gas may cause burns or frostbite.
- Frostbite** : Try to warm up the frozen tissues and seek medical attention.
- Ingestion** : As this product is a gas, refer to the inhalation section.

Over-exposure signs/symptoms

- Eye contact** : No specific data.
- Inhalation** : No specific data.
- Skin contact** : No specific data.
- Ingestion** : No specific data.

Indication of immediate medical attention and special treatment needed, if necessary

- Notes to physician** : Treat symptomatically. Contact poison treatment specialist immediately if large quantities have been ingested or inhaled.
- Specific treatments** : No specific treatment.

Section 4. First aid measures

- Protection of first-aiders** : No action shall be taken involving any personal risk or without suitable training. It may be dangerous to the person providing aid to give mouth-to-mouth resuscitation.

See toxicological information (Section 11)

Section 5. Fire-fighting measures

Extinguishing media

- Suitable extinguishing media** : Use an extinguishing agent suitable for the surrounding fire.
- Unsuitable extinguishing media** : None known.

- Specific hazards arising from the chemical** : Contains gas under pressure. Extremely flammable gas. In a fire or if heated, a pressure increase will occur and the container may burst, with the risk of a subsequent explosion.

- Hazardous thermal decomposition products** : No specific data.

- Special protective actions for fire-fighters** : Promptly isolate the scene by removing all persons from the vicinity of the incident if there is a fire. No action shall be taken involving any personal risk or without suitable training. Contact supplier immediately for specialist advice. Move containers from fire area if this can be done without risk. Use water spray to keep fire-exposed containers cool. If involved in fire, shut off flow immediately if it can be done without risk. If this is impossible, withdraw from area and allow fire to burn. Fight fire from protected location or maximum possible distance. Eliminate all ignition sources if safe to do so.

- Special protective equipment for fire-fighters** : Fire-fighters should wear appropriate protective equipment and self-contained breathing apparatus (SCBA) with a full face-piece operated in positive pressure mode.

Section 6. Accidental release measures

Personal precautions, protective equipment and emergency procedures

- For non-emergency personnel** : Accidental releases pose a serious fire or explosion hazard. No action shall be taken involving any personal risk or without suitable training. Evacuate surrounding areas. Keep unnecessary and unprotected personnel from entering. Shut off all ignition sources. No flares, smoking or flames in hazard area. Avoid breathing gas. Provide adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Put on appropriate personal protective equipment.

- For emergency responders** : If specialized clothing is required to deal with the spillage, take note of any information in Section 8 on suitable and unsuitable materials. See also the information in "For non-emergency personnel".

- Environmental precautions** : Ensure emergency procedures to deal with accidental gas releases are in place to avoid contamination of the environment. Inform the relevant authorities if the product has caused environmental pollution (sewers, waterways, soil or air).

Methods and materials for containment and cleaning up

- Small spill** : Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment.
- Large spill** : Immediately contact emergency personnel. Stop leak if without risk. Use spark-proof tools and explosion-proof equipment. Note: see Section 1 for emergency contact information and Section 13 for waste disposal.

Section 7. Handling and storage

Precautions for safe handling

Protective measures : Put on appropriate personal protective equipment (see Section 8). Contains gas under pressure. Avoid breathing gas. Use only with adequate ventilation. Wear appropriate respirator when ventilation is inadequate. Do not enter storage areas and confined spaces unless adequately ventilated. Do not puncture or incinerate container. Use equipment rated for cylinder pressure. Close valve after each use and when empty. Protect cylinders from physical damage; do not drag, roll, slide, or drop. Use a suitable hand truck for cylinder movement.

Use only non-sparking tools. Avoid contact with eyes, skin and clothing. Empty containers retain product residue and can be hazardous. Store and use away from heat, sparks, open flame or any other ignition source. Use explosion-proof electrical (ventilating, lighting and material handling) equipment.

Advice on general occupational hygiene : Eating, drinking and smoking should be prohibited in areas where this material is handled, stored and processed. Workers should wash hands and face before eating, drinking and smoking. Remove contaminated clothing and protective equipment before entering eating areas. See also Section 8 for additional information on hygiene measures.

Conditions for safe storage, including any incompatibilities : Store in accordance with local regulations. Store in a segregated and approved area. Store away from direct sunlight in a dry, cool and well-ventilated area, away from incompatible materials (see Section 10). Eliminate all ignition sources. Cylinders should be stored upright, with valve protection cap in place, and firmly secured to prevent falling or being knocked over. Cylinder temperatures should not exceed 52 °C (125 °F). Keep container tightly closed and sealed until ready for use. See Section 10 for incompatible materials before handling or use.

Section 8. Exposure controls/personal protection

Control parameters

Occupational exposure limits

Ingredient name	Exposure limits
hydrogen	<p>California PEL for Chemical Contaminants (Table AC-1) (United States). Oxygen Depletion [Asphyxiant].</p> <p>ACGIH TLV (United States, 3/2019). Oxygen Depletion [Asphyxiant]. Explosive potential.</p>

Appropriate engineering controls : Use only with adequate ventilation. Use process enclosures, local exhaust ventilation or other engineering controls to keep worker exposure to airborne contaminants below any recommended or statutory limits. The engineering controls also need to keep gas, vapor or dust concentrations below any lower explosive limits. Use explosion-proof ventilation equipment.

Environmental exposure controls : Emissions from ventilation or work process equipment should be checked to ensure they comply with the requirements of environmental protection legislation. In some cases, fume scrubbers, filters or engineering modifications to the process equipment will be necessary to reduce emissions to acceptable levels.

Individual protection measures

Hygiene measures : Wash hands, forearms and face thoroughly after handling chemical products, before eating, smoking and using the lavatory and at the end of the working period. Appropriate techniques should be used to remove potentially contaminated clothing. Wash contaminated clothing before reusing. Ensure that eyewash stations and safety showers are close to the workstation location.

Section 8. Exposure controls/personal protection

- Eye/face protection** : Safety eyewear complying with an approved standard should be used when a risk assessment indicates this is necessary to avoid exposure to liquid splashes, mists, gases or dusts. If contact is possible, the following protection should be worn, unless the assessment indicates a higher degree of protection: safety glasses with side-shields.
- Skin protection**
- Hand protection** : Chemical-resistant, impervious gloves complying with an approved standard should be worn at all times when handling chemical products if a risk assessment indicates this is necessary. Considering the parameters specified by the glove manufacturer, check during use that the gloves are still retaining their protective properties. It should be noted that the time to breakthrough for any glove material may be different for different glove manufacturers. In the case of mixtures, consisting of several substances, the protection time of the gloves cannot be accurately estimated.
- Body protection** : Personal protective equipment for the body should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product. When there is a risk of ignition from static electricity, wear anti-static protective clothing. For the greatest protection from static discharges, clothing should include anti-static overalls, boots and gloves.
- Other skin protection** : Appropriate footwear and any additional skin protection measures should be selected based on the task being performed and the risks involved and should be approved by a specialist before handling this product.
- Respiratory protection** : Based on the hazard and potential for exposure, select a respirator that meets the appropriate standard or certification. Respirators must be used according to a respiratory protection program to ensure proper fitting, training, and other important aspects of use. Respirator selection must be based on known or anticipated exposure levels, the hazards of the product and the safe working limits of the selected respirator.

Section 9. Physical and chemical properties

Appearance

- Physical state** : Gas
- Color** : Colorless.
- Odor** : Odorless.
- Odor threshold** : Not available.
- pH** : Not available.
- Melting point** : -259.15°C (-434.5°F)
- Boiling point** : -253°C (-423.4°F)
- Critical temperature** : -240.15°C (-400.3°F)
- Flash point** : Not available.
- Evaporation rate** : Not available.
- Flammability (solid, gas)** : Extremely flammable in the presence of the following materials or conditions: oxidizing materials.
- Lower and upper explosive (flammable) limits** : Lower: 4%
Upper: 76%
- Vapor pressure** : Not available.
- Vapor density** : 0.07 (Air = 1) Liquid Density@BP: 4.43 lb/ft³ (70.96 kg/m³)
- Specific Volume (ft³/lb)** : 12.0482
- Gas Density (lb/ft³)** : 0.083
- Relative density** : Not applicable.
- Solubility** : Not available.
- Solubility in water** : Not available.
- Partition coefficient: n-octanol/water** : Not available.
- Auto-ignition temperature** : 500 to 571°C (932 to 1059.8°F)
- Decomposition temperature** : Not available.

Section 9. Physical and chemical properties

Viscosity : Not applicable.

Flow time (ISO 2431) : Not available.

Molecular weight : 2.02 g/mole

Aerosol product

Heat of combustion : -116486080 J/kg

Section 10. Stability and reactivity

Reactivity : No specific test data related to reactivity available for this product or its ingredients.

Chemical stability : The product is stable.

Possibility of hazardous reactions : Under normal conditions of storage and use, hazardous reactions will not occur.

Conditions to avoid : Avoid all possible sources of ignition (spark or flame). Do not pressurize, cut, weld, braze, solder, drill, grind or expose containers to heat or sources of ignition.

Incompatible materials : Oxidizers

Hazardous decomposition products : Under normal conditions of storage and use, hazardous decomposition products should not be produced.

Hazardous polymerization : Under normal conditions of storage and use, hazardous polymerization will not occur.

Section 11. Toxicological information

Information on toxicological effects

Acute toxicity

Not available.

Irritation/Corrosion

Not available.

Sensitization

Not available.

Mutagenicity

Not available.

Carcinogenicity

Not available.

Reproductive toxicity

Not available.

Teratogenicity

Not available.

Specific target organ toxicity (single exposure)

Not available.

Specific target organ toxicity (repeated exposure)

Not available.

Aspiration hazard

Not available.

Section 11. Toxicological information

Information on the likely routes of exposure : Not available.

Potential acute health effects

- Eye contact** : Contact with rapidly expanding gas may cause burns or frostbite.
- Inhalation** : No known significant effects or critical hazards.
- Skin contact** : Contact with rapidly expanding gas may cause burns or frostbite.
- Ingestion** : As this product is a gas, refer to the inhalation section.

Symptoms related to the physical, chemical and toxicological characteristics

- Eye contact** : No specific data.
- Inhalation** : No specific data.
- Skin contact** : No specific data.
- Ingestion** : No specific data.

Delayed and immediate effects and also chronic effects from short and long term exposure

Short term exposure

- Potential immediate effects** : Not available.
- Potential delayed effects** : Not available.

Long term exposure

- Potential immediate effects** : Not available.
- Potential delayed effects** : Not available.

Potential chronic health effects

Not available.

- General** : No known significant effects or critical hazards.
- Carcinogenicity** : No known significant effects or critical hazards.
- Mutagenicity** : No known significant effects or critical hazards.
- Teratogenicity** : No known significant effects or critical hazards.
- Developmental effects** : No known significant effects or critical hazards.
- Fertility effects** : No known significant effects or critical hazards.

Numerical measures of toxicity

Acute toxicity estimates

Not available.

Section 12. Ecological information

Toxicity

Not available.

Persistence and degradability

Not available.

Bioaccumulative potential

Not available.

Section 12. Ecological information

Mobility in soil






Soil/water partition coefficient (K_{oc}) : Not available.

Other adverse effects : No known significant effects or critical hazards.

Section 13. Disposal considerations

Disposal methods : The generation of waste should be avoided or minimized wherever possible. Disposal of this product, solutions and any by-products should at all times comply with the requirements of environmental protection and waste disposal legislation and any regional local authority requirements. Dispose of surplus and non-recyclable products via a licensed waste disposal contractor. Waste should not be disposed of untreated to the sewer unless fully compliant with the requirements of all authorities with jurisdiction. Empty Airgas-owned pressure vessels should be returned to Airgas. Waste packaging should be recycled. Incineration or landfill should only be considered when recycling is not feasible. This material and its container must be disposed of in a safe way. Empty containers or liners may retain some product residues. Do not puncture or incinerate container.

Section 14. Transport information

	DOT	TDG	Mexico	IMDG	IATA
UN number	UN1049	UN1049	UN1049	UN1049	UN1049
UN proper shipping name	HYDROGEN, COMPRESSED	HYDROGEN, COMPRESSED	HYDROGEN COMPRESSED	HYDROGEN, COMPRESSED	HYDROGEN, COMPRESSED
Transport hazard class(es)	2.1 	2.1 	2.1 	2.1 	2.1 
Packing group	-	-	-	-	-
Environmental hazards	No.	No.	No.	No.	No.

“Refer to CFR 49 (or authority having jurisdiction) to determine the information required for shipment of the product.”

Additional information

DOT Classification : **Limited quantity** Yes.
Quantity limitation Passenger aircraft/rail: Forbidden. Cargo aircraft: 150 kg.

TDG Classification : Product classified as per the following sections of the Transportation of Dangerous Goods Regulations: 2.13-2.17 (Class 2).
Explosive Limit and Limited Quantity Index 0.125
ERAP Index 3000
Passenger Carrying Vessel Index Forbidden
Passenger Carrying Road or Rail Index Forbidden

IATA : **Quantity limitation** Passenger and Cargo Aircraft: Forbidden. Cargo Aircraft Only: 150 kg.

Special precautions for user : **Transport within user's premises:** always transport in closed containers that are upright and secure. Ensure that persons transporting the product know what to do in the event of an accident or spillage.

Section 14. Transport information

Transport in bulk according to IMO instruments : Not available.

Section 15. Regulatory information

U.S. Federal regulations : **TSCA 8(a) CDR Exempt/Partial exemption:** This material is listed or exempted.
Clean Air Act (CAA) 112 regulated flammable substances: hydrogen

Clean Air Act Section 112 (b) Hazardous Air Pollutants (HAPs) : Not listed

Clean Air Act Section 602 Class I Substances : Not listed

Clean Air Act Section 602 Class II Substances : Not listed

DEA List I Chemicals (Precursor Chemicals) : Not listed

DEA List II Chemicals (Essential Chemicals) : Not listed

SARA 302/304

Composition/information on ingredients

No products were found.

SARA 304 RQ : Not applicable.

SARA 311/312

Classification : Refer to Section 2: Hazards Identification of this SDS for classification of substance.

State regulations

Massachusetts : This material is listed.

New York : This material is not listed.

New Jersey : This material is listed.

Pennsylvania : This material is listed.

California Prop. 65

This product does not require a Safe Harbor warning under California Prop. 65.

International regulations

Chemical Weapon Convention List Schedules I, II & III Chemicals

Not listed.

Montreal Protocol

Not listed.

Stockholm Convention on Persistent Organic Pollutants

Not listed.

Rotterdam Convention on Prior Informed Consent (PIC)

Not listed.

UNECE Aarhus Protocol on POPs and Heavy Metals

Not listed.

Inventory list

Australia : This material is listed or exempted.

Canada : This material is listed or exempted.

China : This material is listed or exempted.

Europe : This material is listed or exempted.

Section 15. Regulatory information

Japan	: Japan inventory (ENCS): Not determined. Japan inventory (ISHL): Not determined.
New Zealand	: This material is listed or exempted.
Philippines	: This material is listed or exempted.
Republic of Korea	: This material is listed or exempted.
Taiwan	: This material is listed or exempted.
Thailand	: Not determined.
Turkey	: Not determined.
United States	: This material is active or exempted.
Viet Nam	: This material is listed or exempted.

Section 16. Other information

Hazardous Material Information System (U.S.A.)

Health	/	1
Flammability		4
Physical hazards		3

Caution: HMIS® ratings are based on a 0-4 rating scale, with 0 representing minimal hazards or risks, and 4 representing significant hazards or risks. Although HMIS® ratings and the associated label are not required on SDSs or products leaving a facility under 29 CFR 1910.1200, the preparer may choose to provide them. HMIS® ratings are to be used with a fully implemented HMIS® program. HMIS® is a registered trademark and service mark of the American Coatings Association, Inc.

The customer is responsible for determining the PPE code for this material. For more information on HMIS® Personal Protective Equipment (PPE) codes, consult the HMIS® Implementation Manual.

National Fire Protection Association (U.S.A.)



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Copyright ©2001, National Fire Protection Association, Quincy, MA 02269. This warning system is intended to be interpreted and applied only by properly trained individuals to identify fire, health and reactivity hazards of chemicals. The user is referred to certain limited number of chemicals with recommended classifications in NFPA 49 and NFPA 325, which would be used as a guideline only. Whether the chemicals are classified by NFPA or not, anyone using the 704 systems to classify chemicals does so at their own risk.

Procedure used to derive the classification

Classification	Justification
FLAMMABLE GASES - Category 1 GASES UNDER PRESSURE - Compressed gas	Expert judgment According to package

History

Date of printing	: 11/15/2020
Date of issue/Date of revision	: 11/15/2020
Date of previous issue	: 9/27/2018
Version	: 1.01

Section 16. Other information

Key to abbreviations

- : ATE = Acute Toxicity Estimate
- BCF = Bioconcentration Factor
- GHS = Globally Harmonized System of Classification and Labelling of Chemicals
- IATA = International Air Transport Association
- IBC = Intermediate Bulk Container
- IMDG = International Maritime Dangerous Goods
- LogPow = logarithm of the octanol/water partition coefficient
- MARPOL = International Convention for the Prevention of Pollution From Ships, 1973 as modified by the Protocol of 1978. ("Marpol" = marine pollution)
- UN = United Nations

References

- : Not available.

Notice to reader

To the best of our knowledge, the information contained herein is accurate. However, neither the above-named supplier, nor any of its subsidiaries, assumes any liability whatsoever for the accuracy or completeness of the information contained herein.

Final determination of suitability of any material is the sole responsibility of the user. All materials may present unknown hazards and should be used with caution. Although certain hazards are described herein, we cannot guarantee that these are the only hazards that exist.

Safety Data Sheet

according to 29CFR1910/1200 and GHS Rev. 3

Effective date : 01.08.2015

Page 1 of 8

Methanol, Lab Grade, 4L

SECTION 1 : Identification of the substance/mixture and of the supplier

Product name : Methanol, Lab Grade, 4L

Manufacturer/Supplier Trade name:

Manufacturer/Supplier Article number: S25426A

Recommended uses of the product and uses restrictions on use:

Manufacturer Details:

AquaPhoenix Scientific
9 Barnhart Drive, Hanover, PA 17331

Supplier Details:

Fisher Science Education
15 Jet View Drive, Rochester, NY 14624

Emergency telephone number:

Fisher Science Education Emergency Telephone No.: 800-535-5053

SECTION 2 : Hazards identification

Classification of the substance or mixture:



Flammable

Flammable liquids, category 2



Toxic

Acute toxicity (oral, dermal, inhalation), category 3



Health hazard

Specific target organ toxicity following single exposure, category 1

AcTox Dermal. 3

Flammable liq. 2

AcTox Oral. 3

AcTox Inhaln. 3

Stot SE. 1

Signal word :Danger

Hazard statements:

Highly flammable liquid and vapour

Toxic if swallowed

Toxic in contact with skin

Toxic if inhaled

Causes damage to organs

Precautionary statements:

If medical advice is needed, have product container or label at hand

Keep out of reach of children

Read label before use

Safety Data Sheet

according to 29CFR1910/1200 and GHS Rev. 3

Effective date : 01.08.2015

Page 2 of 8

Methanol, Lab Grade, 4L

Wear protective gloves/protective clothing/eye protection/face protection
Wash skin thoroughly after handling
Do not eat, drink or smoke when using this product
Avoid breathing dust/fume/gas/mist/vapours/spray
Keep away from heat/sparks/open flames/hot surfaces. No smoking
Do not breathe dust/fume/gas/mist/vapours/spray
Specific treatment (see supplemental first aid instructions on this label)
IF ON SKIN: Wash with soap and water
Call a POISON CENTER or doctor/physician if you feel unwell
Specific measures (see supplemental first aid instructions on this label)
Take off contaminated clothing and wash before reuse
Wash contaminated clothing before reuse
IF SWALLOWED: Immediately call a POISON CENTER or doctor/physician
IF exposed: Call a POISON CENTER or doctor/physician
IF INHALED: Remove victim to fresh air and keep at rest in a position comfortable for breathing
Store locked up
Store in a well ventilated place. Keep cool
Dispose of contents and container as instructed in Section 13

Other Non-GHS Classification:

WHMIS



NFPA/HMIS



NFPA SCALE (0-4)

Health	2
Flammability	3
Physical Hazard	0
Personal Protection	X

HMIS RATINGS (0-4)

SECTION 3 : Composition/information on ingredients

Ingredients:

CAS 67-56-1

Methanol

>90 %

Safety Data Sheet

according to 29CFR1910/1200 and GHS Rev. 3

Effective date : 01.08.2015

Page 3 of 8

Methanol, Lab Grade, 4L

Percentages are by weight

SECTION 4 : First aid measures

Description of first aid measures

After inhalation: Move exposed individual to fresh air. Loosen clothing as necessary and position individual in a comfortable position. Get medical assistance. If breathing is difficult, give oxygen

After skin contact: Wash affected area with soap and water. Rinse/flush exposed skin gently using water for 15-20 minutes. Seek medical attention if irritation persists or if concerned.

After eye contact: Protect unexposed eye. Rinse or flush eye gently with water for at least 15-20 minutes, lifting upper and lower lids. Seek medical attention if irritation persists or if concerned

After swallowing: Rinse mouth thoroughly. Do not induce vomiting. Have exposed individual drink sips of water. Dilute mouth with water or milk after rinsing. Get medical assistance.

Most important symptoms and effects, both acute and delayed:

Poison. Toxic by ingestion, absorption through skin and inhalation, potentially causing irreversible effects. Irritating to eyes, skin, and respiratory tract. Irritation- all routes of exposure. Shortness of breath. Nausea. Headache. May be fatal or cause blindness if swallowed. Cannot be made non-poisonous. May cause gastrointestinal irritation, vomiting, and diarrhea. Central nervous system disorders. Skin disorders, preexisting eye disorders, gastrointestinal tract; Toxic: danger of very serious irreversible effects by inhalation, ingestion or absorption through skin. Experiments have shown reproductive toxicity effects on laboratory animals. May cause adverse kidney and liver effects

Indication of any immediate medical attention and special treatment needed:

If seeking medical attention, provide SDS document to physician. Physician should treat symptomatically.

SECTION 5 : Firefighting measures

Extinguishing media

Suitable extinguishing agents: Dry chemical, foam, dry sand, or Carbon Dioxide. Water spray can keep containers cool.

For safety reasons unsuitable extinguishing agents: Water may be ineffective.

Special hazards arising from the substance or mixture:

Risk of ignition. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back. Containers may explode when heated

Advice for firefighters:

Protective equipment: Wear protective eyewear, gloves, and clothing. Refer to Section 8.

Additional information (precautions): Remove all sources of ignition. Avoid contact with skin, eyes, and clothing. Ensure adequate ventilation. Take precautions against static discharge.

SECTION 6 : Accidental release measures

Personal precautions, protective equipment and emergency procedures:

Use spark-proof tools and explosion-proof equipment. Provide exhaust ventilation or other engineering controls to keep the airborne concentrations of vapor and mists below the applicable workplace exposure limits (Occupational Exposure Limits-OELs) indicated above. Ensure adequate ventilation.

Environmental precautions:

Prevent from reaching drains, sewer or waterway. Should not be released into environment.

Methods and material for containment and cleaning up:

If necessary use trained response staff or contractor. Remove all sources of ignition. Contain spillage and then

Safety Data Sheet

according to 29CFR1910/1200 and GHS Rev. 3

Effective date : 01.08.2015

Page 4 of 8

Methanol, Lab Grade, 4L

collect. Do not flush to sewer. Absorb with a noncombustible absorbent material such as sand or earth and containerize for disposal. Ventilate area of leak or spill. Use spark-proof tools and explosion-proof equipment. Follow proper disposal methods. Refer to Section 13.

Reference to other sections:

SECTION 7 : Handling and storage

Precautions for safe handling:

Use in a chemical fume hood. Wash hands before breaks and immediately after handling the product. Avoid contact with skin, eyes, and clothing. Take precautions against static discharge.

Conditions for safe storage, including any incompatibilities:

Store in a cool location. Provide ventilation for containers. Avoid storage near extreme heat, ignition sources or open flame. Keep container tightly sealed. Store with like hazards. Protect from freezing and physical damage.

SECTION 8 : Exposure controls/personal protection



Control Parameters:

67-56-1, Methanol, ACGIH: 250 ppm STEL; 200 ppm TWA
67-56-1, Methanol, NIOSH: 250 ppm STEL; 325 mg/m³ STEL
67-56-1, Methanol, NIOSH: 200 ppm TWA; 260 mg/m³ TWA

Appropriate Engineering controls: Emergency eye wash fountains and safety showers should be available in the immediate vicinity of use or handling. Ensure that dust-handling systems (exhaust ducts, dust collectors, vessels, and processing equipment) are designed to prevent the escape of dust into the work area.

Respiratory protection: Use in a chemical fume hood. If exposure limit is exceeded, a full-face respirator with organic cartridge may be worn.

Protection of skin: Select glove material impermeable and resistant to the substance. Select glove material based on rates of diffusion and degradation.

Eye protection: Safety glasses with side shields or goggles.

General hygienic measures: Wash hands before breaks and at the end of work. Avoid contact with the eyes and skin. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Perform routine housekeeping.

SECTION 9 : Physical and chemical properties

Appearance (physical state,color):	Clear colorless liquid	Explosion limit lower: Explosion limit upper:	6 31
Odor:	Alcohol	Vapor pressure:	128 hPa @ 20°C
Odor threshold:	Not Available	Vapor density:	1.11
pH-value:	Not Available	Relative density:	0.79
Melting/Freezing point:	-98°C	Solubilities:	Miscible at 20 °C

Safety Data Sheet

according to 29CFR1910/1200 and GHS Rev. 3

Effective date : 01.08.2015

Page 5 of 8

Methanol, Lab Grade, 4L

Boiling point/Boiling range:	64.7°C @ 760mmHg	Partition coefficient (n-octanol/water):	Not Available
Flash point (closed cup):	12°C	Auto/Self-ignition temperature:	455°C
Evaporation rate:	5.2	Decomposition temperature:	Not Available
Flammability (solid,gaseous):	Flammable	Viscosity:	a. Kinematic:Not Available b. Dynamic: Not Available
Density: Not Available			

SECTION 10 : Stability and reactivity

Reactivity:Vapours may form explosive mixture with air.

Chemical stability:Stable under normal conditions.

Possible hazardous reactions:None under normal processing.

Conditions to avoid:Excess heat, Incompatible Materials, flames, or sparks.

Incompatible materials: Oxidizing agents, reducing agents, alkali metals, acids, sodium, potassium, metals as powders, acid chlorides, acid anhydrides, powdered magnesium, and aluminum.

Hazardous decomposition products:carbon monoxide, formaldehyde.

SECTION 11 : Toxicological information

Acute Toxicity:		
Dermal:	(rabbit)	LD-50 15800 mg/kg
Oral:	(rat)	LD-50 5628 mg/kg
Inhalation:	(rat)	LC-50 130,7 mg/l
Chronic Toxicity: No additional information.		
Corrosion Irritation:		
Ocular:		Irritating to eyes
Dermal:		Irritating to skin
Sensitization:		No additional information.
Single Target Organ (STOT):		Classified as causing damage to organs: Eyes, skin, optic nerve, gastrointestinal tract, central nervous system, respiratory system, liver, spleen, kidney, blood
Numerical Measures:		No additional information.
Carcinogenicity:		Teratogenicity : has occurred in experimental animals.
Mutagenicity:		Mutagenetic effects have occurred in experimental animals.

Safety Data Sheet

according to 29CFR1910/1200 and GHS Rev. 3

Effective date : 01.08.2015

Page 6 of 8

Methanol, Lab Grade, 4L

Reproductive Toxicity:

Developmental Effects (Immediate/Delayed) have occurred in experimental animals

SECTION 12 : Ecological information

Ecotoxicity

Freshwater Fish: 96 Hr LC50 Pimephales promelas: 28200 mg/L

Freshwater Fish: 96 Hr LC50 Oncorhynchus mykiss: 19500 - 20700 mg/L

Freshwater Fish: 96 Hr LC50 Pimephales promelas: >100 mg/L

Freshwater Fish: 96 Hr LC50 Oncorhynchus mykiss: 18 - 20 mL/L

Freshwater Fish: 96 Hr LC50 Lepomis macrochirus: 13500 - 17600 mg/L

Persistence and degradability: Not persistent.

Bioaccumulative potential: Not Bioaccumulative.

Mobility in soil: Aqueous solution has high mobility in soil.

Other adverse effects:

SECTION 13 : Disposal considerations

Waste disposal recommendations:

Methanol RCRA waste code U154. Do not allow product to reach sewage system or open water. It is the responsibility of the waste generator to properly characterize all waste materials according to applicable regulatory entities (US 40CFR262.11). Absorb with a noncombustible absorbent material such as sand or earth and containerize for disposal. Provide ventilation. Have fire extinguishing agent available in case of fire. Eliminate all sources of ignition. Use spark-proof tools and explosion-proof equipment. Chemical waste generators must determine whether a discarded chemical is classified as a hazardous waste. Chemical waste generators must also consult local, regional, and national hazardous waste regulations. Ensure complete and accurate classification.

SECTION 14 : Transport information

UN-Number

UN1230

UN proper shipping name

Methanol

Transport hazard class(es)



Class:

3 Flammable liquids



Class:

6.1 Toxic substances

Packing group: II

Environmental hazard:

Transport in bulk:

Special precautions for user:

SECTION 15 : Regulatory information

Safety Data Sheet

according to 29CFR1910/1200 and GHS Rev. 3

Effective date : 01.08.2015

Page 7 of 8

Methanol, Lab Grade, 4L

United States (USA)

SARA Section 311/312 (Specific toxic chemical listings):

Acute, Chronic, Fire

SARA Section 313 (Specific toxic chemical listings):

67-56-1 Methanol

RCRA (hazardous waste code):

67-56-1 Methanol RCRA waste code U154

TSCA (Toxic Substances Control Act):

All ingredients are listed.

CERCLA (Comprehensive Environmental Response, Compensation, and Liability Act):

67-56-1 Methanol 5000 lbs

Proposition 65 (California):

Chemicals known to cause cancer:

None of the ingredients is listed

Chemicals known to cause reproductive toxicity for females:

None of the ingredients is listed

Chemicals known to cause reproductive toxicity for males:

None of the ingredients is listed

Chemicals known to cause developmental toxicity:

67-56-1 Methanol

Canada

Canadian Domestic Substances List (DSL):

All ingredients are listed.

Canadian NPRI Ingredient Disclosure list (limit 0.1%):

None of the ingredients is listed

Canadian NPRI Ingredient Disclosure list (limit 1%):

67-56-1 Methanol

SECTION 16 : Other information

This product has been classified in accordance with hazard criteria of the Controlled Products Regulations and the SDS contains all the information required by the Controlled Products Regulations. Note: The responsibility to provide a safe workplace remains with the user. The user should consider the health hazards and safety information contained herein as a guide and should take those precautions required in an individual operation to instruct employees and develop work practice procedures for a safe work environment. The information contained herein is, to the best of our knowledge and belief, accurate. However, since the conditions of handling and use are beyond our control, we make no guarantee of results, and assume no liability for damages incurred by the use of this material. It is the responsibility of the user to comply with all applicable laws and regulations applicable to this material.

GHS Full Text Phrases:

Abbreviations and acronyms:

IMDG: International Maritime Code for Dangerous Goods

PNEC: Predicted No-Effect Concentration (REACH)

Safety Data Sheet

according to 29CFR1910/1200 and GHS Rev. 3

Effective date : 01.08.2015

Page 8 of 8

Methanol, Lab Grade, 4L

CFR: Code of Federal Regulations (USA)

SARA: Superfund Amendments and Reauthorization Act (USA)

RCRA: Resource Conservation and Recovery Act (USA)

TSCA: Toxic Substances Control Act (USA)

NPRI: National Pollutant Release Inventory (Canada)

DOT: US Department of Transportation

IATA: International Air Transport Association

GHS: Globally Harmonized System of Classification and Labelling of Chemicals

ACGIH: American Conference of Governmental Industrial Hygienists

CAS: Chemical Abstracts Service (division of the American Chemical Society)

NFPA: National Fire Protection Association (USA)

HMIS: Hazardous Materials Identification System (USA)

WHMIS: Workplace Hazardous Materials Information System (Canada)

DNEL: Derived No-Effect Level (REACH)

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Last updated : 03.27.2015