Dimethyl Carbonate Production Using Carbon Dioxide

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Executive Summary

This report presents a conceptual process design and analysis for a carbon-negative dimethyl carbonate (DMC) plant with a production capacity of 100 kta. The analysis covers a distillation system, isobaric CSTR, heat exchanger network, and compression system. The proposed plant aims to sell 100 kta of polymer-grade DMC at $1100/MT, using a feed of 50 kta ethylene oxide (EO) at $1250/MT, 70 kta methanol (MeOH) at $600/MT, and 50 kta CO_2 at $45/MT. The reaction produces ethylene glycol (EG) as a coproduct and 2-methoxyethanol (ME) as a byproduct. EG can be sold at $500/MT, while ME is discarded due to lack of a large-scale market. The maximum economic potential analysis indicates a value of $31 MM/year with EG purification and sale, and $2 MM/year without, highlighting the importance of EG in the process. Our analysis shows that a 100 m³ CSTR operating at 50 bar and 140°C offers the best economic potential, achieving ~96% single-pass reactor conversion and ~98% DMC/EO selectivity. The plant produces 0.7 kg of CO_2 and requires 33 MJ of energy per kg of DMC synthesized. The CSTR and associated equipment assume a 12-year operational lifespan and a 3-year construction period. Reactor and separation conditions were optimized for maximum net present value (NPV). The optimized economic analysis yields an NPV of -$6.7 MM, a total capital investment (TCI) of $44.1 MM, and an internal rate of return (IRR) of 14.1%. Given the negative NPV, alternative locations were considered for better profitability. Constructing the plant in the European Economic Area could increase the NPV to $90 MM, with a TCI of $44.1MM and an IRR of 48%, due to favorable market prices and the carbon credit system in Europe. Using original contract prices but implementing the carbon credit in Europe would result in an NPV of $9 MM.

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1 Introduction

1.1 Motivation and Background

Recent divestment from fossil fuel companies by the University of California have allowed for a new pool of funds to be utilized for investment by the University of California Retirement Plan (UCRP). These funds have the potential to be used for sustainable chemical manufacturing, with a main focus on bio/CO_2 based feedstock sources. We plan to include potential future economic incentives for using CO_2 as a feedstock and investing in a carbon consuming process. We expect that the CO_2 tax that is increasing around the world[2] will raise the price of products that are produced from CO_2 emitting plants. This further increases the economic potential of operating a carbon negative process.

We at Chemical Investment Advisors (CIA) have developed a sustainable chemical plant for the production of dimethyl carbonate (DMC) using CO_2 as a feedstock source. This proposed chemical plant will produce DMC at 100kta for an estimated $1100/MT and ethylene glycol (EG), a byproduct, at an estimated $500/MT. The preliminary design demonstrates the use of a catalyzed, stirred slurry tank reactor for the production of DMC has a maximum economic potential of $31 MM/year. From this estimation, we determine that a 100 kta DMC plant design & economic analysis is warranted due to the potential profits.

1.2 Market Analysis

Our team has completed an extensive market analysis that considers industry reports of all main economic factors in this chemical plant to provide validity of investment. We have determined that carbon credits are expected to be quickly introduced into US markets considering the expectation of $100-400 billion to be invested in 2030 for CO_2 removal capacity[2]. Another consideration is seen in the European carbon trade market where "credits" are ~$80/MT currently[3,10]. The market for CO_2 sequestration is only expected to grow as legislation and regulations move towards taxing more heavily on emissions and giving more credit to the consumption of CO_2.

The overall DMC market has remained stable over the past half decade with similar expectations into the future based on the increase of DMC demand. The value for DMC is estimated at $1000/MT as of September 2023[4]. We are assuming a contract selling price of $1100/MT[1] for DMC. This market price can be expected to increase due the future carbon emission taxes that will affect incumbent DMC production facilities. This may lead to increased sale prices and make our designed process more competitive.

The ethylene glycol market has seen steady growth in demand and value across the past 4 years with the most recent price being ~$870/MT as of September 2021[5]. We are assuming a contract selling value of $500/MT[1]. Our analysts expect EG to hover at this price into the near future based on historical trends[5]. EG is a vital byproduct of the process chemistry and preliminary estimates of maximum economic potential yield a revenue of $31 MM/year, as opposed to an economic potential of $2 MM/year without the sale of EG.

The estimated buying price for ethylene oxide (EO) in the current market has seen very little change in the US at a value of \$1080/MT over the past 2 years as of 2019[6]. We are assuming a contract purchasing price of \$1250/MT[1].

The most recent methanol spot prices are \$660/MT as of June 2024[7]. We are assuming a contract purchasing price of \$600/MT[1]. The market value has been observed to be steady over the past year and is expected to maintain this price over the lifetime of our projected plant operation. We believe that due to carbon taxes and credits increasing, preliminary DMC production plant design is warranted.

1.3 Reaction Chemistry

The following three reactions below represent an accurate model for the kinetics under various reaction conditions ranging from 50-150 bar and temperatures ranging from 80-140°C. The first reaction is instantaneous leading reaction 2 and 3 to determine the overall rate. The forward rate of the second reaction is ~50 times larger than that of the reverse reaction, and 100 times greater than that of the third reaction.

$$EO \ + \ CO_2 \rightarrow EC \qquad\qquad \Delta H_{rxn}= \text{-61 KJ/mol} \qquad (1)$$

$$EC \ + \ MeOH \rightleftharpoons DMC \ + \ EG \qquad \Delta H_{rxn}= \text{-54 KJ/mol} \qquad (2)$$

$$EG \ + \ MeOH \rightarrow ME \ + \ CO_2 \qquad \Delta H_{rxn}= \text{-55 KJ/mol} \qquad (3)$$

With EO = ethylene oxide, EC = ethylene carbonate, MeOH = methanol, DMC = dimethyl carbonate, EG = ethylene glycol, and ME = 2-methoxyethanol. The overall reaction is exothermic, seen from the exclusively negative enthalpies of reaction. Additionally, the kinetic models, rate expressions, and temperature dependence for isothermal and isobaric reactor operation are explicitly outlined in Appendix C.

2 Conceptual Design

The conceptual design of this process includes reactor simulation in MATLAB, Aspen HYSYS, and Aspen Plus. The simulation is then optimized with respect to economic parameters. We examine five main process alternatives: high pressure distillation, pressure swing distillation, a separate hydrolysis reactor, multiple reactors in series, and more complex tower design (side draws). We determine optimal reactor design conditions for our assumed contract prices based on project NPV. We then further analyze the profitability of the plant if it were to be built in Europe based on current European market values for feed and product chemicals along with existing CO_2 credit markets.
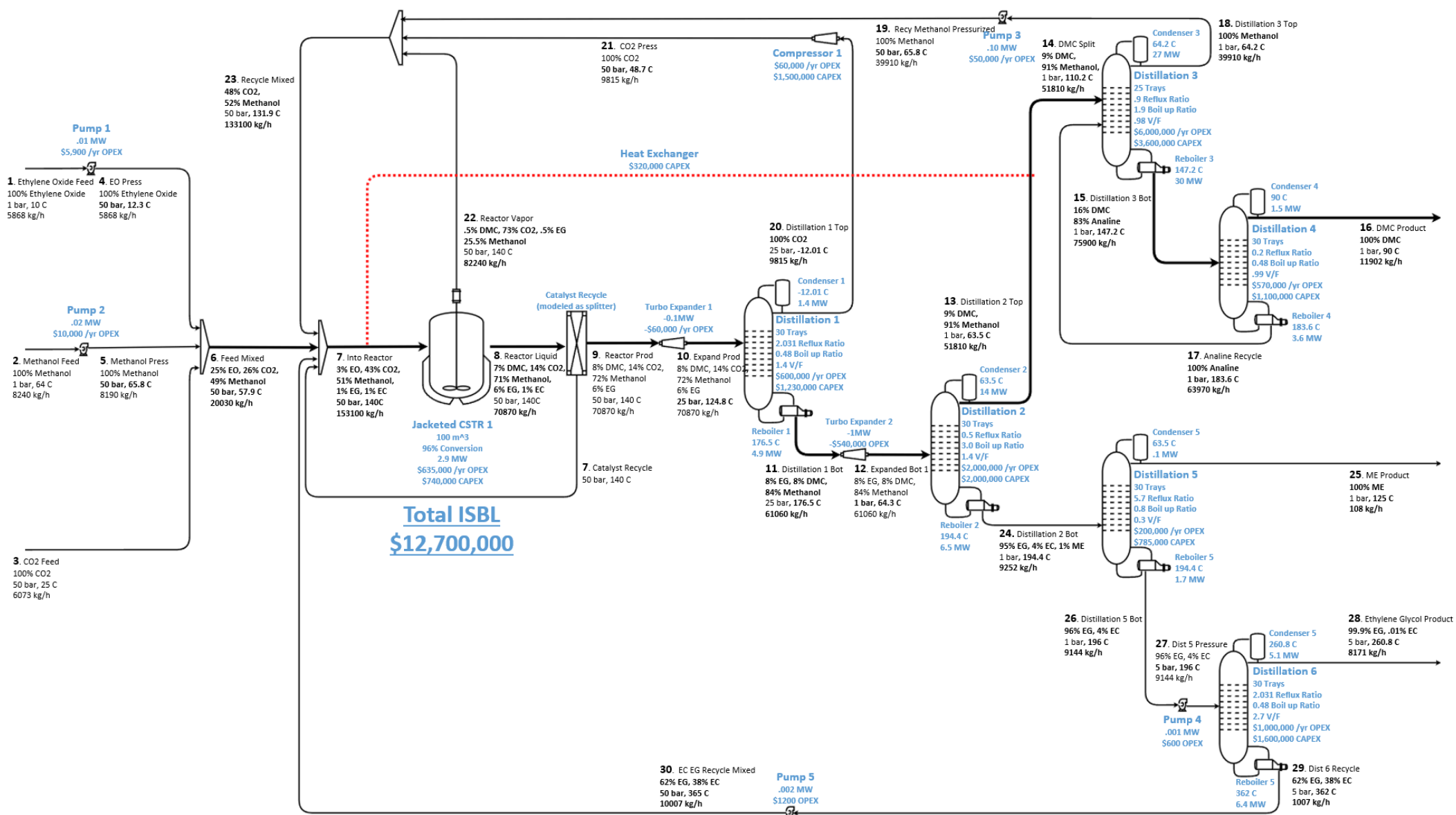
Figure 1. Process flow sheet of our optimized DMC production where a positive dollar amount shows costs, and a negative dollar amount shows value of energy from expanding

Stream Name	Stream Number	Vapor Fraction	Temperature [C]	Pressure [kPa]	Mass Flow [kg/h]
Ethylene Oxide Feed	1	0.0	10	100	5868
Methanol Feed	2	0.0	64	100	8240
CO$_2$ Feed	3	1.0	25	5000	6073
EO Press	4	0.0	12	5000	5868
Methanol Pressurized	5	0.0	66	5000	8240
Feed Mixed	6	0.0	58	5000	20030
Into Reactor	7	0.4	140	5000	153100
Reactor Liquid	8	0.0	140	5000	70870
Reactor Prod	9	0.0	140	5000	70870
Expanded Prod	10	0.1	126	2500	70870
Distillation 1 Bot	11	0.0	177	2500	61060
Expanded Bot 1	12	0.5	64	100	61060
Distillation 2 Top	13	0.0	63	100	51810
DMC Split	14	0.0	110	100	51810
Distillation 3 Bot	15	0.0	147	100	75900
DMC Product	16	0.0	90	100	11902
Aniline Recycle	17	0.0	184	100	63970
Distillation 3 Top	18	0.0	64	100	39910
Recy Methanol Pressurized	19	0.0	66	5000	39910
Distillation 1 Top	20	1.0	-12	2500	9815
CO2 Press	21	1.0	49	5000	9815
Reactor Vapor	22	1.0	140	5000	82240
Recycle Mixed	23	0.4	134	5000	133100
Distillation 2 Bot	24	0.0	194	100	9252
ME Product	25	0.0	124	100	108
Distillation 5 Bot	26	0.0	196	100	9144
Dist 5 Pressure	27	0.0	196	500	9144
Ethylene Glycol Product	28	0.0	261	500	8171
Dist 6 Recycle	29	0.0	362	500	1007
EC EG Recycle Mixed	30	0.0	365	5000	1007

Stream Name	Stream Number	Ethylene-Glycol	Ethylene-Carbonate	Ethylene-Oxide	Dimethyl-Carbonate	Carbon-Dioxide	Methanol	2-Methoxyethanol	Aniline
Ethylene Oxide Feed	1	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
Methanol Feed	2	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00
CO$_2$ Feed	3	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
EO Press	4	0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
Methanol Pressurized	5	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00
Feed Mixed	6	0.00	0.00	0.25	0.00	0.26	0.49	0.00	0.00
Into Reactor	7	0.00	0.00	0.03	0.00	0.45	0.51	0.00	0.00
Reactor Liquid	8	0.08	0.00	0.00	0.08	0.13	0.71	0.00	0.00
Reactor Prod	9	0.08	0.00	0.00	0.08	0.13	0.71	0.00	0.00
Expanded Prod	10	0.08	0.00	0.00	0.08	0.13	0.71	0.00	0.00
Distillation 1 Bot	11	0.09	0.00	0.00	0.09	0.00	0.82	0.00	0.00
Expanded Bot 1	12	0.09	0.00	0.00	0.09	0.00	0.82	0.00	0.00
Distillation 2 Top	13	0.00	0.00	0.00	0.10	0.00	0.90	0.00	0.00
DMC Split	14	0.00	0.00	0.00	0.10	0.00	0.90	0.00	0.00
Distillation 3 Bot	15	0.00	0.00	0.00	0.16	0.00	0.00	0.00	0.84
DMC Product	16	0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00
Aniline Recycle	17	0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
Distillation 3 Top	18	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00
Recy Methanol Pressurized	19	0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00
Distillation 1 Top	20	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
CO$_2$ Press	21	0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
Reactor Vapor	22	0.00	0.00	0.00	0.01	0.73	0.26	0.00	0.00
Recycle Mixed	23	0.01	0.00	0.00	0.00	0.48	0.51	0.00	0.00
Distillation 2 Bot	24	0.95	0.04	0.00	0.00	0.00	0.00	0.01	0.00
ME Product	25	0.01	0.00	0.00	0.00	0.00	0.00	0.99	0.00
Distillation 5 Bot	26	0.96	0.04	0.00	0.00	0.00	0.00	0.00	0.00
Dist 5 Pressure	27	0.96	0.04	0.00	0.00	0.00	0.00	0.00	0.00
Ethylene Glycol Product	28	1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Dist 6 Recycle	29	0.62	0.38	0.00	0.00	0.00	0.00	0.00	0.00
EC EG Recycle Mixed	30	0.62	0.38	0.00	0.00	0.00	0.00	0.00	0.00

Table 1. Master stream table containing mass flows, mole percent, temperature, pressure, and vapor fraction for streams in the plant.

*all values on this page are given in mole percent

2.1 Process Overview & Simulation

The proposed process design involves optimizing reactor conditions, designing a distillation and separation system, and heat integration. The process utilizes a stirred slurry tank reactor to produce dimethyl carbonate (DMC) and ethylene glycol (EG) from carbon dioxide (CO_2), methanol (MeOH), and ethylene oxide (EO). For effective reaction kinetics, the feed must contain excess CO_2 and MeOH, maintaining a 13:1 molar ratio of CO_2 to EO and a 15:1 molar ratio of MeOH to EO. The reactor uses 1:1 mass ratios of catalysts potassium iodide and potassium carbonate, with 1 gram of catalyst mixture for every 50 mL of EO/methanol solution.

To reduce feed costs, CO_2, MeOH, and the reaction intermediate ethylene carbonate (EC) are recycled. The stirred slurry tank is modeled as a continuous stirred-tank reactor (CSTR) in MATLAB, using various rate expressions (detailed in Appendix C) for both isothermal and isobaric conditions. This simulation allows us to determine crucial relationships, such as the product selectivity of DMC/EO versus conversion, and to identify optimal reaction conditions that are expected to yield the highest NPV.

Simulation results are validated against those obtained from Aspen HYSYS and Aspen Plus, ensuring they align closely with the conceptual design. Once optimal reactor conditions are established, a practical separation system, including a series of six distillation columns, is designed. Additionally, a heat exchanger is designed to cool the feed stream to the required reactor temperature. Steam is used to vaporize material in the reboilers, while cooling water condenses the distillate in the condensers. We then considered the sequestration costs of CO_2 produced from steam production to maintain carbon a negative preliminary design. A detailed cost analysis is then conducted based on the finalized design to assess project feasibility, with results compared to initial MATLAB simulation projections.

Key assumptions in the MATLAB conceptual design include modeling supercritical CO_2 as a liquid and assuming the liquid within the CSTR is incompressible at reactor conditions. While this assumption is not accurate, especially below the supercritical point of CO_2 (73.8 bar and 31.1°C), it helps create a predictive model for outlet concentrations. Comparison with Aspen HYSYS shows that this assumption does not significantly affect reactor conversion, with only a ~0.2% conversion difference when reactors of the same volume are modeled using different methods. This is likely because only the first reaction involves CO_2 and is modeled as an instantaneous reaction in MATLAB with 100% conversion, while Aspen HYSYS uses a 100% conversion reactor.

2.1.1 Key Design Parameters

In this stage of process development we are able to vary reactor temperature, volume, and pressure. We determine these optimal parameters by systematically varying different reactor volumes within our MATLAB simulation and maximizing economic parameters.

2.2 Process Alternatives

2.2.1 Higher Pressure CO_2 Distillation/Reaction

Higher pressure CO_2 distillation was considered to minimize pressure differential of the CO_2 needing repressurization[8]. Using the CSTR vent allows for recycling CO_2 at the operating pressure of 50 bar, which reduces recompression cost significantly. Operating the CO_2 distillation column at full reflux reduced condenser temperature to 60°C, allowing for the use of cooling water. Recompression of CO_2 to 50 bar is prohibitively expensive; therefore, we analyzed operating the column at pressures from 5 to 50 bar. We determined that 25 bar was the highest safe pressure to avoid the risk of high-pressure CO_2 ruptures and asphyxiation. NPV analysis on different CO_2 distillation pressures are shown explicitly in Section 2.5.

2.2.2 Pressure Swing for DMC Methanol Azeotrope

We examined two ways to break the DMC-methanol azeotrope: pressure swing distillation and using an aniline entrainer. Pressure swing would eliminate the need for another distillation tower but was incredibly energy-intensive. This could be achieved by running columns 2 and 3 at 11.5 bar to split the azeotrope[11] without the need for column 4. This method required a high-stage column with prohibitively high reboiler and condenser operating expenses. This analysis favors an aniline entrainer extractive distillation column as more cost-effective.

2.2.3 Hydrolysis of EC to EG

Breaking the ethylene carbonate (EC) and ethylene glycol (EG) azeotrope could be done by increasing distillation pressure or via hydrolysis. The XY vapor curve for EC and EG showed that, at our effluent concentrations, the mixture lies to the right of the distillation boundary (Appendix A Figure A11) at 5 bar, which allows for cost effective distillation[13]. Hydrolyzing EC to EG in a CSTR was considered but would prevent recycling of unreacted EC, reducing selectivity for DMC production. Preliminary HYSYS simulation and costing indicated this would decrease NPV by ~$20 million, even as we accounted for adding water, recycling base, reacting adiabatically in a CSTR, and using a small distillation column to recycle the water. We believed that this was overly complex compared to our alternative, along with being less profitable. We therefore opted to run a pressurized tower at 5 bar to split EG from EC.

2.2.4 Levenspiel Analysis

Levenspiel analysis indicated that multiple CSTRs in series would reduce the required volume of the reactors by 20 m^3 to reach the required conversion. However, this reduction in volume is not justified due to the economics at this scale (multiple small heat exchangers and CSTRs are more expensive than one large jacketed CSTR). We decided against this approach because the project statement specifically tasked us with using a CSTR for this reaction.

2.2.5 Complex Tower Design

We also explored complex tower designs with integrated side draws and recycles between coupled distillation towers to optimize energy usage. This design aimed to ensure that components would not spend significant time in the condenser and reboiler, thus optimizing energy efficiency. Further energy optimization between these columns was deemed unnecessary at this stage. We wanted to maintain flexibility, allowing this design to be adaptable if we

identified more significant changes in other areas, rather than committing to an overly specific optimized column design.

2.3 MATLAB CSTR Simulation & Optimization

2.3.1 Continuous Stirred Slurry Tank Simulation

We modeled the continuous stirred slurry tank as either an isobaric or isothermal CSTR, depending on kinetics, and utilized the design algorithm outlined in Appendix D[1]. The conversion of EC at different reactor volumes as a result of the MATLAB and HYSYS simulation is shown in Figure 2A and 2C, respectively. We then determine the selectivity of DMC/EO vs. conversion for the MATLAB and HYSYS simulations as shown in Figure 2B and 2D, respectively. Selectivity versus conversion for either the MATLAB or HYSYS simulation did not show appreciable changes for different temperatures or pressures. A comprehensive compilation of the design variables is shown in Appendix A, Figures A.1-A.6.
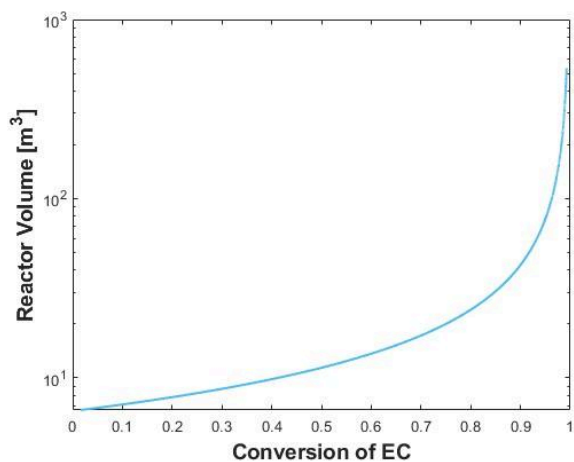
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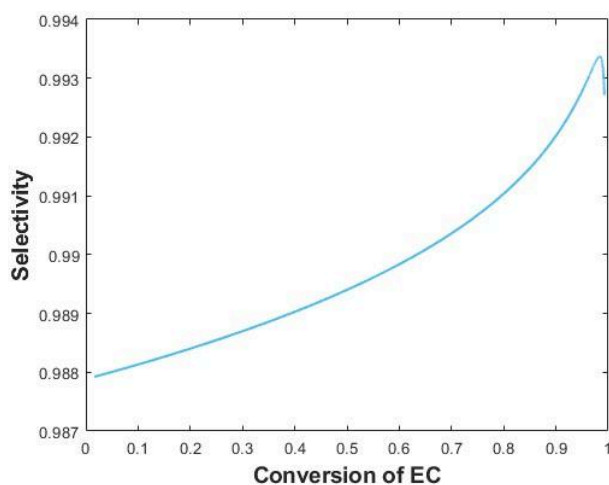
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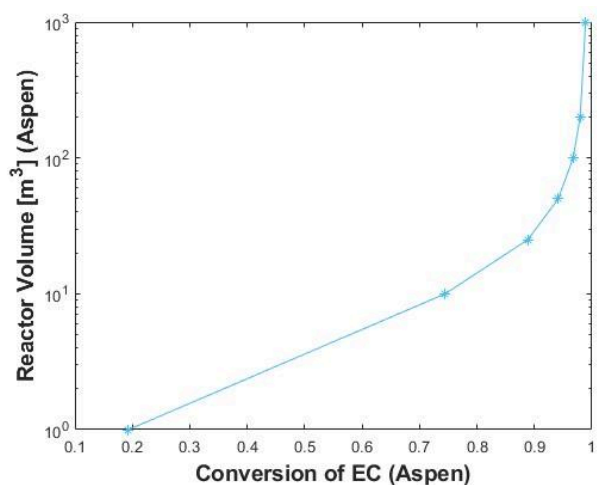
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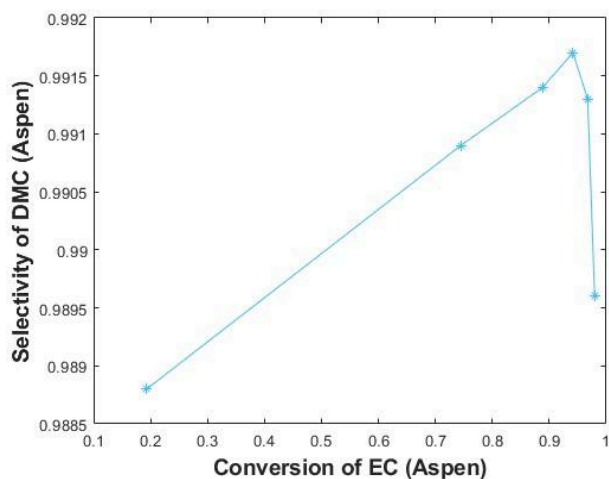
2D.

Figure 2. 2A. Reactor conversion of limiting reactant at different CSTR volumes with operating conditions of T = 140 C, P = 50 bar based on MATLAB simulation.
2B. Selectivity of DMC/EO vs. conversion at different operating conditions based on MATLAB simulation. As the reaction conversion increases, the selectivity increases until a maximum is reached at 0.96, followed by a sharp decline in selectivity.
2C. Reactor conversion of limiting reactant at different CSTR volumes with operating conditions of T = 140 C, P = 50 bar based on Aspen HYSYS simulation.
2D. Selectivity of DMC/EO vs. conversion at T = 140ºC and P = 50 bar based on select points in Aspen HYSYS simulation.

2.3.2 Net Present Value Reactor Optimization

We considered the cost of feed methanol, CO_2, ethylene oxide, the CSTR, approximate compressor/pump electricity and a simplified separation system for NPV calculations utilizing MATLAB results. The costing of the simplified separation system utilizes a scaling of the minimum thermodynamic work required to separate components into pure streams by 35. Capital and operating expenses are determined based on the scaled minimum thermodynamic work and scaled by $0.75/W. A detailed outline for this estimation is shown in Appendix E.

Optimal values for key design parameters are found via economic analysis and optimization. Specifically, reactor temperature, pressure, and volume are optimized with respect to NPV of the plant at the end of the 15 year project lifetime (3 years of construction and 12 years of operation). Optimal CSTR conditions include an operating temperature of 140ºC, reaction pressure of 50 bar, and a volume of 100 m³ (corresponding to a single pass conversion of 96 %). These conditions utilize the isothermal set of reaction kinetics outlined in Appendix C. The optimal NPV with a simplified separation system was found to be ~ - $ 12.5 MM and is determined by Figure 3A. We then vary the CSTR pressure from 50 to 150 bar and observe that the optimal NPV occurs with a reactor pressure of 50 bar.
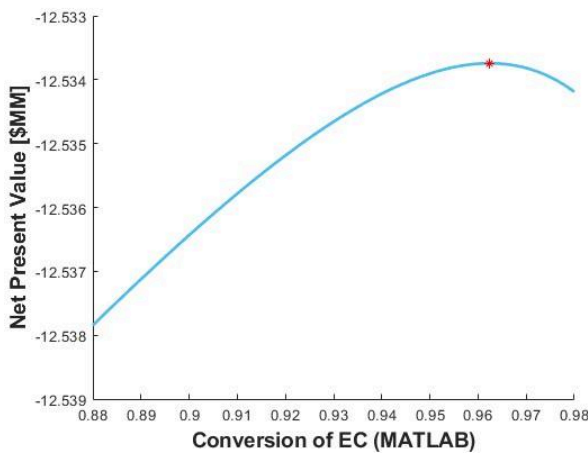
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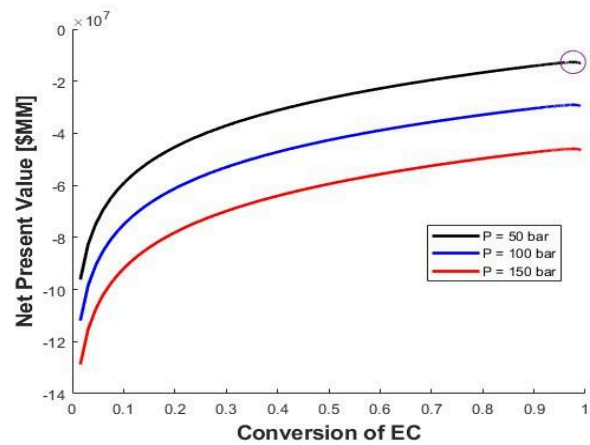
3B.

Figure 3. 3A. NPV[$MM] vs. reactor conversion for a CSTR with an operating pressure of 50 bar and temperature of 140ºC based on MATLAB simulation.
3B. NPV [$MM] vs. reactor conversion for a CSTR with various operating pressures from 50 to 150 bar and a constant temperature of 140ºC based on MATLAB simulation.

Costing of each of these parameters is described explicitly with their associated cost correlations in Appendix E and optimal reactor parameters are valued in Section 3. At this stage of design we do not consider a purge, however, future designs past FEL-1 will likely require one.

The following subsections utilize the optimal CSTR volume and conditions as a starting point for a detailed design of the separation system and heat exchanger network as part of our conceptual design. The conditions and volume are then verified against a more rigorous NPV calculation including realistic operating and capital expenses for compressors/expanders and distillation towers. Further considerations of realistic NPV calculations include varying reactor volume and distillation pressure for the Aspen HYSYS simulation.

2.3.3 Separation System Design & Optimization

The separation system includes six distillation columns using pressure swing distillation and aniline as an entrainer to break EG/EC and DMC/MeOH azeotropes, respectively. The reactor effluent is vented and recycled at reactor pressure, removing a large amount of CO_2 and reducing the need for recompression. The remaining liquid effluent is expanded to 25 bar via a turboexpander and sent to the first distillation tower, where the remaining CO_2 is separated into vapor (via a full reflux condenser), recompressed to 50 bar, and sent to the recycle stream.

The remaining reactor effluent is then split into two streams containing the two azeotropes via distillation tower 2. This splitting procedure is used to reduce energy expenditure associated with splitting the azeotropes by having dedicated tower systems for each azeotrope. The DMC/MeOH stream is sent to an extractive distillation column (3) with a 1:1 molar ratio of aniline to feed. This breaks the azeotrope and allows for the removal and recycling of the remaining MeOH. The DMC/aniline mixture is then sent to a final tower (4) where DMC is separated and condensed at 99.9 wt% purity for polymer-grade DMC, while the aniline is recycled to the extractive distillation tower. The bottom of tower 2 is sent to tower 5, which removes the remaining MeOH and ME from the EG/EC mixture. The bottoms of tower 5, containing the EC/EG mixture, are pumped to 5 bar, allowing the azeotrope to break in tower 6, and a 99.5 wt% of EG is purified from the condenser. The distillate of tower 5, composed of ME with trace MeOH, is discarded. A table showing V/F, reflux & boilup ratio, and trays is presented in Table 2.

Distillation Column	V/F (mol basis)	Reflux Ratio	Boilup Ratio	Trays
1	1.4	2.0	0.5	30 Trays
2	1.4	0.5	3.0	30 Trays
3	1.0	0.9	1.9	25 Trays
4	1.0	0.2	0.5	30 Trays
5	0.3	5.7	0.8	30 Trays
6	2.7	2.0	40.8	30 Trays

Table 2. Vapor rate/feed flow, reflux ratio, boilup ratio, and number of trays for each distillation column within the separation system.

2.4 Energy Integration and Balances

2.4.1 Heater Exchangers

Our design includes one process heat exchanger which exchanges heat between the feed with the distillate of tower 2. This heat exchanger has an area of 3400 ft^2 and ensures that the feed is kept at the correct operating temperature of 140 °C. Costing and duty for this heat exchanger is shown in Section 3.1.

2.4.2 Separation System Energy Requirements

The energy requirements for the distillation system contains most of the operating and capital expenses of the plant due to the large number of towers and large flows needed to be heated and cooled. Steam is used to vaporize material in the reboilers of the towers while cooling water ($3/GJ) is used to condense the distillate streams. Saturated steam prices at various pressures and temperatures were taken from Douglas & Malone[13].

2.5 Process Alternatives

We systematically varied the reactor volume and distillation pressure of the CO_2 removal tower and observed that the maximum NPV for this process occurs at a reactor volume of 100 m^3 and distillation pressure of 25 bar. The optimal reactor volume found from Aspen HYSYS is 100 m^3 which agrees with the MATLAB conceptual design. Distillation pressure was varied only in Aspen HYSYS and we determined that the pressure of 25 bar is the most optimal due to the significantly reduced compression requirements for the recycled CO_2. Illustrations of the change in NPV versus reactor conversion and the pressure of the CO_2 removal column are shown in Figure 4A and 4B, respectively.
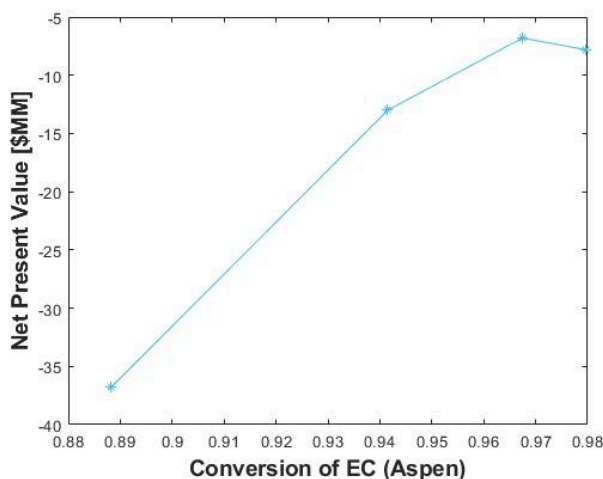
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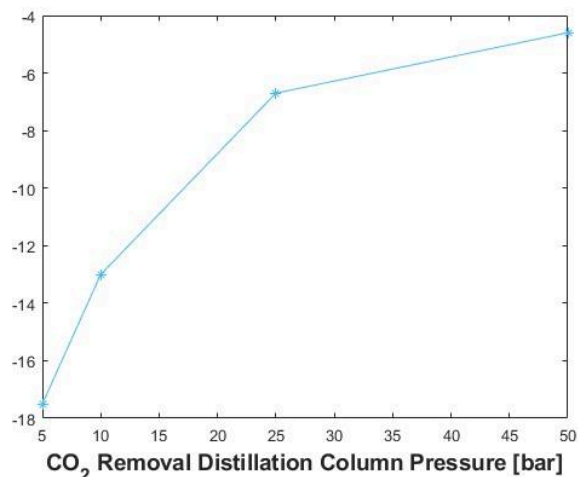
4B.

Figure 4. 4A. NPV[$MM] vs. reactor conversion for a CSTR with an operating pressure of 50 bar and temperature of 140°C based on Aspen HYSYS simulation.
 4B. NPV [$MM] vs. distillation pressure for the CO_2 removal tower with a constant CSTR volume of 100 m^3 based on Aspen HYSYS simulation.

3 Economic Analysis

3.1 Equipment List

The conceptual process includes 10 pieces of equipment, costed based on correlations in Appendix E, using a Marshall and Swift index of 1800 for the year 2024[1]. Pumps are excluded due to their minimal power requirements and capital expenses. Detailed calculations for each piece of equipment are outlined in Appendix E.

The CSTR is modeled as a single large, well-mixed tank with a monodisperse residence time and is rated for an operating pressure of 50 bar with a volume of 100 m³. Stainless steel was selected for all vessels because of its resistance to corrosion from the feed and products at high pressures. The reactor cooler is costed as a shell and tube heat exchanger for simplicity.

Distillation capital expenses (CAPEX) include tray costing, pressure vessels, and heat exchangers for the reboiler and condenser[14]. Heat exchangers are the most expensive component, contributing the most to the distillation system CAPEX. All tower internals are stainless steel, with the tower assembled using sieve trays at 24-inch spacing. The system of six distillation columns accounts for $10 million of our ISBL. Table 3 contains descriptions of all of the considered equipment in this design.

Equipment Name	Description	Material	Total Duty [MW]	OPEX [$MM/yr]	CAPEX [$MM]
CSTR	Pressure vessel + agitator + jacketed heat exchanger	SS	2.8	0.6	0.7
Distillation Column 1	CO_2 removal	SS	6.3	0.6	1.2
Distillation Column 2	DMC/MeOH + EG/EC/ME split	SS	20.5	2.0	2.0
Distillation Column 3	Extractive distillation of DMC/Aniline from DMC/MeOH	SS	57	6.0	3.6
Distillation Column 4	DMC/Aninline split	SS	5.1	0.6	1.1
Distillation Column 5	ME split from EG/EC	SS	1.8	0.2	0.7
Distillation Column 6	EG/EC split at 5 bar	SS	11.5	1.0	1.6
Heat Exchanger	Cools feed to reactor temperature with tower 2 bottoms	SS	6	~	0.3
Compressor	Recompresses CO_2 from 25 bar to 50 bar for recycle	SS	0.12	0.06	1.5
Turboexpander	Expands CSTR effluent from 50 bar to 25 bar	SS	0.12	-0.06	~

Table 3. Equipment table including description, material of construction, duty [MW], and estimated capex and opex.

3.2 Fixed-Capital Summary

The fixed capital cost estimate of this project is extremely important as it provides a reasonable estimate for the upfront investment costs that the plant will have. The ISBL that is contained in this section will consider the total cost of procurement and installation associated with each piece of equipment. These calculations include compressors, distillation towers, heat exchangers, and the reactor.

The total ISBL cost for our process is $12.7 MM. This consists of one heat exchanger and full separation system with specific costing as shown in Table 3 in section 3.1. The fraction of each of these pieces of equipment in the ISBL is shown on the pie chart shown in Figure 5. A preliminary value for the outside battery limit (OSBL) was estimated at 40% of the ISBL[14]. A comprehensive ISBL and OSBL calculation and further description is shown in Appendix E.
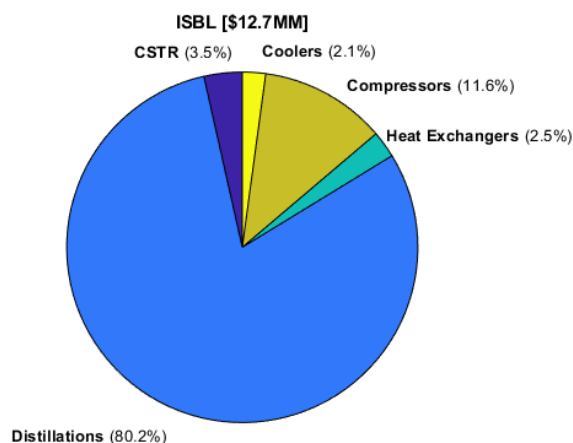
Figure 5. Total $12.7 MM ISBL pie chart for proposed process

Total fixed capital cost (TFCC) was approximately 227% of the ISBL. The TFCC is estimated to be $29 MM for a plant. The TFCC includes ISBL, OSBL (40% of ISBL), a contingency (25% of ISBL+OSBL), and indirect costs (30% of contingency+ISBL+OSBL). The total capital investment for this plant is $44.1 MM which includes the working capital for the plant. These assumptions are used to provide an early estimate based on preliminary equipment costing. Economic modeling requires more detailed cost correlations which is outside the scope of this report. This economic model is described in detail in Appendix F.

3.3 Discounted Cash Flow Analysis

Two discounted cash flow analyses were conducted over the lifetime of the plant after determining all capital and operating expenses. The first case examined assumed contract prices as shown in Appendix F. The second case examined current European market prices[12] mentioned in section 1.2 and is shown in Appendix F. For this calculation, we considered a 3 year construction period, 12 year plant operating life, and an enterprise rate of 15% per year. As well, we assumed a tax rate of 27%, an administration rate of 5% of revenues, and assumed a 10 year linear depreciation model for equipment and a salvage value of 5% of the TFCC for the plant[1].

This discounted cash flow can be translated to an NPV over each year of the project and gives a general estimate for the value gained at each year depending on plant lifetime. Figure 6 shows a comparison of the two NPV vs project lifetime we calculated. Figure 6A considers assumed contract selling prices and excludes carbon credits, and Figure 6B considers real European market values and the inclusion of carbon credit for the preliminary design. This alternative location is discussed further in section 3.5.

6A.

6B.
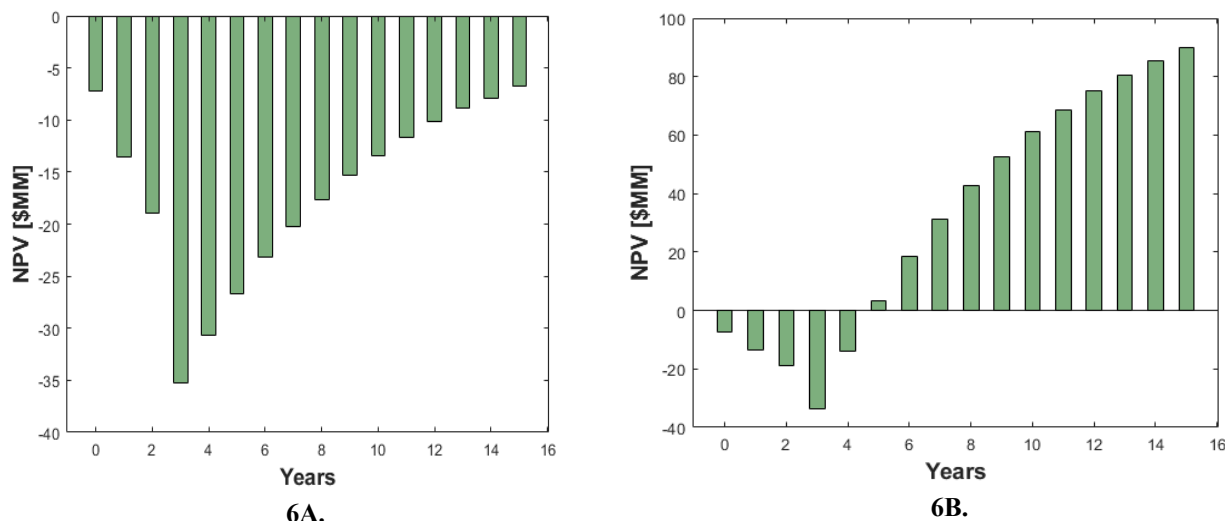
Figure 6. 6A. NPV versus project lifetime assumed contract prices excluding carbon credits
6B. Current European market values including carbon credits

3.4 Profitability Metrics and Analysis

3.4.1 NPV, IRR, and Sensitivity Analysis

The overall profitability of this conceptual design is impacted by costs of feedstock and selling prices of products. However, it is significantly affected by parameters such as the tax on CO_2 sequestration, and the feedstock price of CO_2. A pie chart depicting the fractions of each operating cost is shown in Figure 7. Additionally, a tornado plot for a sensitivity analysis is shown in Figure 8A with tabulated variations shown in Figure 8B.
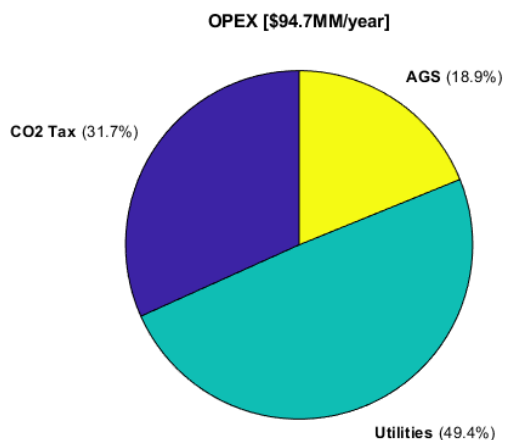
Figure 7. Pie chart of overall plant operating expenses. Utilities for heating and cooling show the greatest influence on operating expenses.
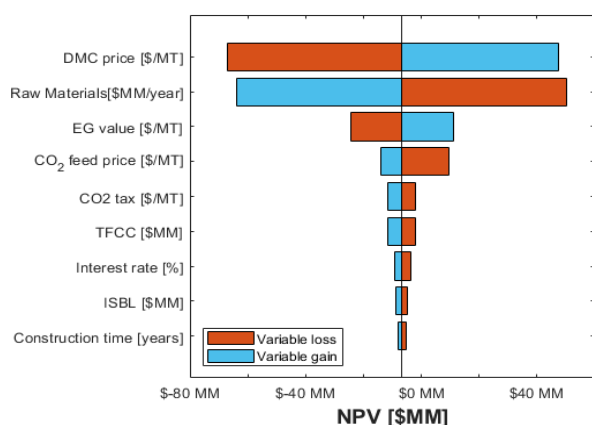
Variable	Variance	Base Case
DMC Price [$/MT]	± 20%	1100
Raw Material Cost [$MM/year]	± 20%	105.1
Ethylene Glycol Price [$/MT]	± 20%	500
CO2 Stock Price [$/MT]	+55 - 120	45
CO2 tax [$/MT]	± 20%	125
TFCC [$MM]	± 20%	28.9
Interest Rate [%]	± 2 points	15
ISBL [$MM]	± 20%	12.7
Construction Time [years]	± 1 year	3

8A.   **8B.**

Figure 8. 8A Sensitivity analysis tornado plot of selected variables deemed important to NPV and accompanying table showing base case value and variation for each variable.
8B. Table showing the variables of choice for the sensitivity analysis with their base case value and range of variation

We performed a sensitivity analysis comparing a large range of potential factors that we deemed important to the profitability of this conceptual design. These calculations were done with both MATLAB and the excel economic CFD(refer to Appendix F) to determine the effect on NPV from changes in these chosen factors. From the tornado plot we can see that the most important factors are the overall raw material cost and the selling price of DMC. The minimum price of DMC was found to be $1127/MT for a NPV of 0. If a CO_2 credit of $50/MT (net CO_2 price of -$5/MT) is given the NPV reaches 0. These large effects on NPV are intuitive as it considers the main product revenue and the main operating costs. However, the sale price of byproduct EG and the CO_2 feedstock specifically have a large impact on NPV. The CO_2 feedstock is of particular interest since we varied it considering the potential for carbon credits at the value of $80/MT[9]. This is seen as the "loss" in variable value for CO_2 feed price in the tornado plot. All other variables that we considered to be most important to profitability for the plant showed little impact on project NPV.

3.4.2 Monte Carlo Simulation

The sensitivity analysis provides valuable insights into our design. However, in practice, our design would be influenced by numerous factors changing simultaneously in either positive or negative ways. To address this, we used a Monte Carlo simulation of our sensitivity analysis on our base case, modeling how we expect our NPV to change by varying each selected variable simultaneously in the sensitivity analysis. The sampling distributions corresponding to each of these cumulative probabilities are shown in Appendix A.7 and A.9, respectively.
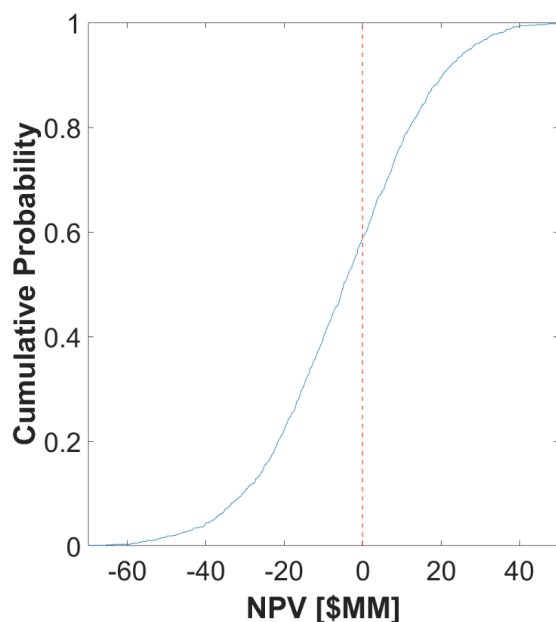
9A.
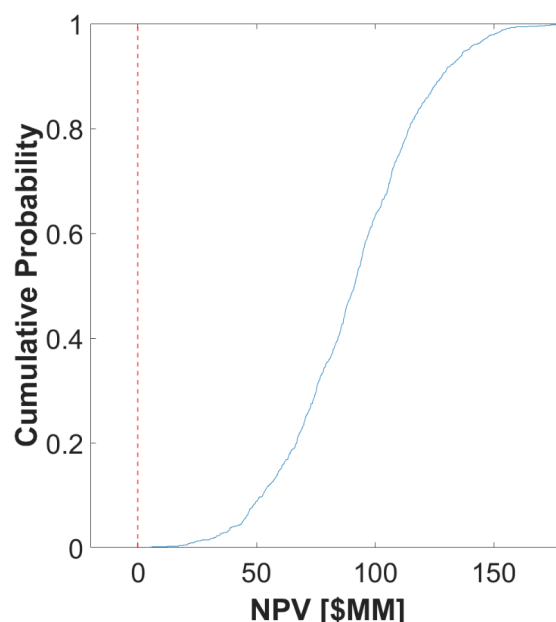
9B.

Figure 9. 9A. The cumulative probability with assumed contract prices.
9B. The cumulative probability with European market prices.

As shown in Figure 9A, there is a 60% chance of a negative NPV with the assumed contract prices and CO_2 taxes. However, in Figure 9B, there is a 99% chance of a positive NPV if we build our plant in Europe.

3.5 Plant Profitability in Europe

We considered the potential of constructing this chemical plant in Europe to take advantage of the carbon credit system and better feed/product price differentials. Pricing values and assumptions are described in Section 2.5. Because the proposed process is carbon negative, we are able to capitalize on the carbon credit market present in Europe at this time with a CO_2 credit value of ~$80/MT[9].

As well, with legislation on carbon emissions and carbon credits likely to enter the industrial world in the near future, we can assume that we will take on a significant amount of carbon credits which further increases expected NPV for this project if constructed in Europe[3].

4 HAZOP and Environmental Impact

The most dangerous aspect of this plant is the high-pressure CO_2, which poses a risk of asphyxiation to plant workers if leaks occur, especially under high pressure. To mitigate this, we limited the CO_2 distillation column pressure to 25 bar. Methanol is highly flammable and, at high pressure, can reach its auto-ignition limit, as shown in Appendix H. EO is highly reactive with a very high auto-ignition point, requiring rigorous safety measures to be implemented while handling EO. A HAZOP analysis for all unit steps is provided in Appendix B, outlining other potential risks and their mitigation strategies.

Sustainability is a key focus, with efforts to enhance utilization of carbon credits, and ongoing research and development for more efficient processes.

By consuming CO_2, the plant can capitalize on carbon credit systems, particularly in Europe, where carbon credits can significantly improve economic viability. Future plans could include integrating renewable energy sources such as solar or wind to further reduce the carbon footprint. Ongoing research will explore more efficient reaction pathways, alternative raw materials, and advanced separation technologies to continuously improve the environmental performance of the plant.

5 Conclusion

This process design and analysis for a 100 kta DMC production facility estimates an NPV of -$6.7 MM if constructed in the US. This assumes the given contract selling and purchasing prices of EO, MeOH, CO_2, DMC, and EG as outlined in Section 1.2. However, if we adjust the prices to current European market values and include carbon credits, the NPV of the plant rises to $90 MM. It is important to note that the profitability of this plant is heavily dependent on the sale of EG as a coproduct. The proposed design features a CSTR with a 100 m³ volume, operating at 140°C and 50 bar, with a single-pass conversion of 96%. Preliminary economic analysis indicates a total capital investment (TCI) of $44.1 MM, with an IRR of 14.1% for the US plant, increasing to 48% if constructed in Europe, while keeping TCI constant.

This economic potential is supported by a detailed market analysis, showing steady demand for DMC and EG, alongside an in-depth review of reaction chemistry and process simulations via MATLAB, Aspen HYSYS, and Aspen Plus. Energy requirements and environmental considerations are addressed, with an estimated energy requirement of 33 MJ per kg of DMC and 0.7 kg of CO_2 produced per kg of DMC produced. The CO_2 sequestration in conjunction with a CO_2 feed makes this plant carbon negative, allowing capitalization on carbon credit systems in certain economies.

This analysis acknowledges the limitations of a preliminary design and suggests further optimization, including exploration of reaction chemistries at lower pressures, the potential of multiple CSTRs in series, and incorporation of a complex distillation tower design. We recommend building this plant in Europe under the given assumptions. However, it is critical to verify contract pricing for feedstock chemicals and that product sale prices align with current market values in Europe to ensure profitability before proceeding with further analysis.

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Appendix

A - Additional Figures
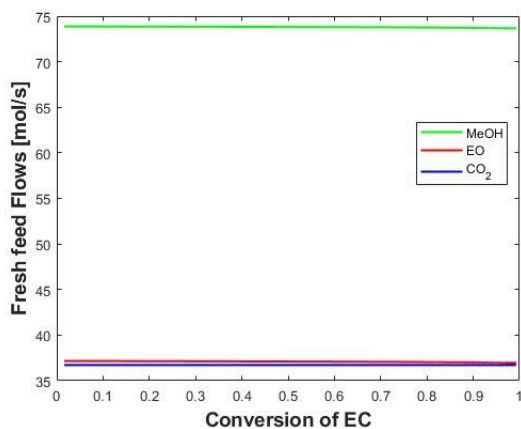
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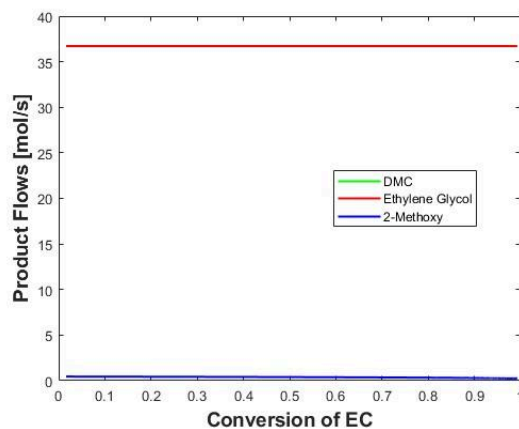
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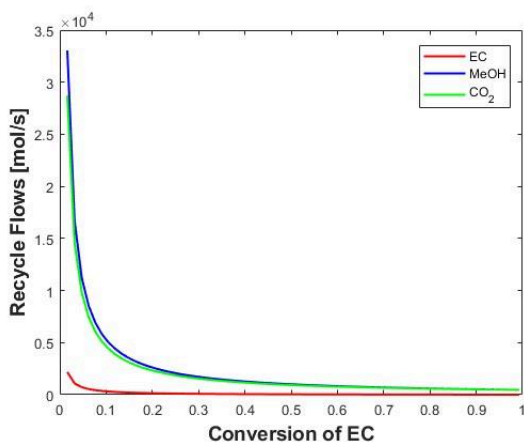
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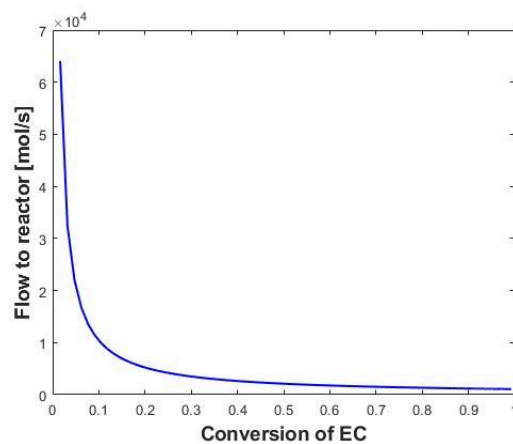
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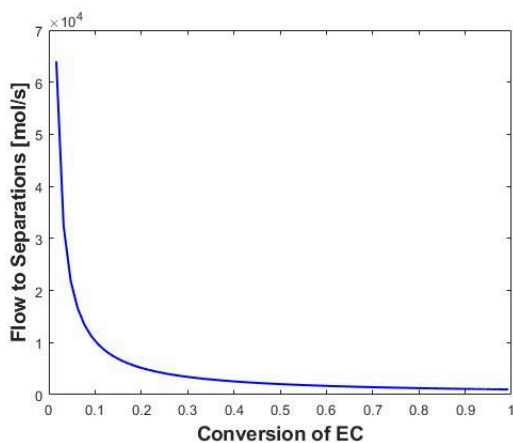
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A6.

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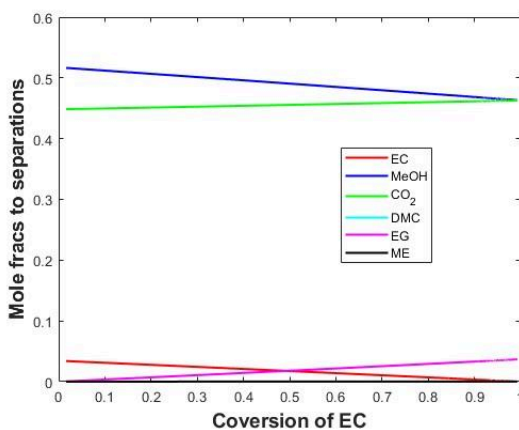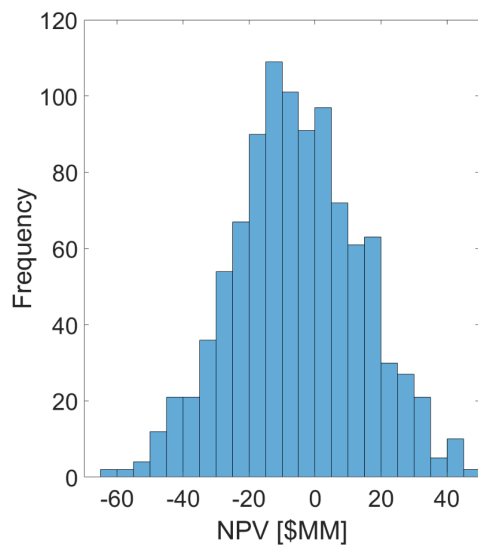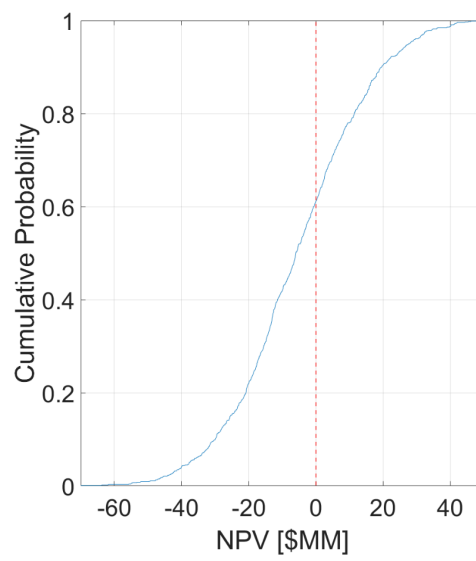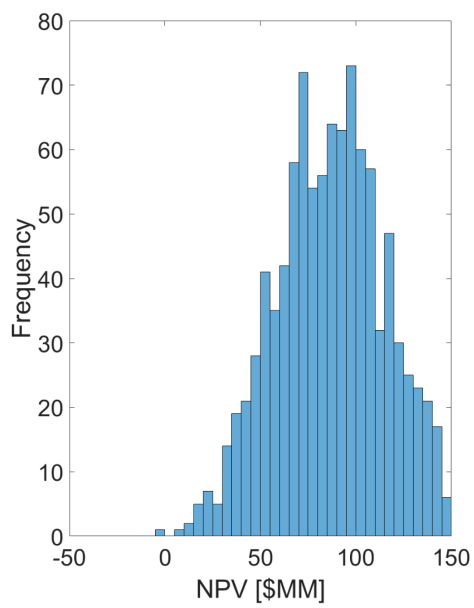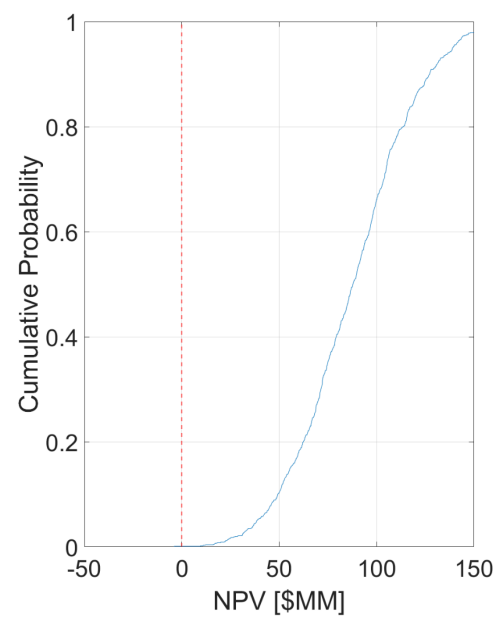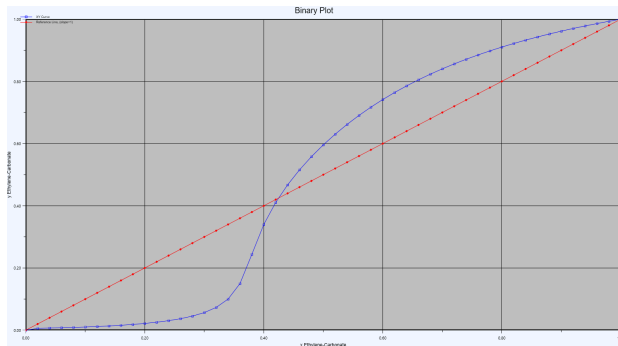
B - Relevant Physical Properties

Property	Ethylene Oxide	Carbon Dioxide	Ethylene Carbonate	Methanol	Dimethyl Carbonate	Ethylene Glycol	2–methox yethanol
Molecular Formula	C_2H_4O	CO_2	$C_3H_4O_3$	CH_3OH	$C_3H_6O_3$	$C_2H_6O_2$	$C_3H_8O_2$
Molecular Weight (g/mol)	44.05	44.01	88.06	32.04	90.08	62.07	76.09
Boiling Point (°C)	10.7	-78.5	242	64.7	90	197.3	124.6
Melting Point (°C)	-111.9	-56.6	34	-97.6	2	-12.9	-85.1
Density (kg/m³ at STP)	1.52	1.98	1.321	0.791	1.07	1.113	0.966
Critical Temperature (°C)	9.3	31.1	-	239	344	197.4	-
Critical Pressure (MPa)	5.04	7.38	-	8.09	5.59	6.98	-
Vapor Pressure at 25°C (kPa)	47.1	517	0.0001	127.6	0.27	0.14	0.11
Specific Gravity (relative to air)	1.52	1.52	-	1.11	-	1.11	-

Solubility in Water (mg/L at STP)	Miscible	1690	Negligible	Miscible	Negligible	Miscible	Miscible
Odor	Sweet, ether-like	Odorless	Faint odor	Slight, pleasant	Odorless	Slightly sweet	Mild, ether-like
Flammability	Highly flammable	Non-flammable	Flammable	Highly flammable	Flammable	Non-flammable	Flammable
Explosive Limits in Air (vol %)	3.0 - 100	5 - 15.3	-	6 - 36.5	3.4 - 17.3	3.2 - 15.1	-
Autoignition Temp. (°C)	429	609	-	470	465	410	-
Toxicity	Highly toxic	Not toxic	Low toxicity	Toxic	Low toxicity	Low toxicity	Toxic
CAS Number	75-21-8	124-38-9	96-49-1	67-56-1	616-38-6	107-21-1	109-86-4
Viscosity (μPa·s at 0°C)	230.6	-	3.29	0.59	-	18.5	5.37
Heat of Combustion (MJ/kg)	-	-	-	22.7	-	-	-

C - Thermodynamics and Reaction Models
C.1 - Reaction Kinetics

$$EO + CO_2 \rightarrow EC \tag{1}$$

$$EC + 2\,MeOH \rightleftharpoons DMC + EG \tag{2}$$

$$EC + MeOH \rightarrow ME + CO_2 \tag{3}$$

$$r_{2,f} = k_{2,f}\, C_{EC}^{0.8} \tag{4}$$

$$r_{2,r} = k_{2,r}\, C_{DMC} C_{EG} \tag{5}$$

$$r_3 = k_3\, C_{EC} \tag{6}$$

$$k_{2,f} = 6.59 \times 10^2 \exp\left(-37,200/RT\right) \tag{7}$$

$$k_{2,r} = 1.19 \times 10^4 \exp\left(-53,700/RT\right) \tag{8}$$

$$k_3 = 1.89 \times 10^6 \exp\left(-82,400/RT\right) \tag{9}$$

$$k_{2,f} = 0.013 \qquad\qquad 50 < \rho < 246.82 \text{ g L}^{-1} \tag{10}$$

$$k_{2,f} = 0.02486 - 4.943 \times 10^{-5}\rho \qquad\qquad \rho > 246.82 \text{ g L}^{-1} \tag{11}$$

$$k_{2,r} = 0.01486\, \rho^{-0.873} \qquad\qquad \rho > 50 \text{ g L}^{-1} \tag{12}$$

$$k_3 = 3.014 \times 10^{-4} \exp\left(-5.99 \times 10^{-3}\rho\right) \qquad\qquad \rho > 50 \text{ g L}^{-1} \tag{13}$$

For the production of DMC from CO_2 we decided on incorporating kinetic rate equations to enhance the yield of desired species where concentrations are in mol L^{-1}, activation energies are in J mol^{-1}, temperatures are in K, and rate constants are in whatever units needed to give rate in mol L^{-1} s^{-1}. This method consisted of determining which set of rate constants to use for an optimal reactor condition where equations 7-9 represent the isobaric kinetic model, and equations 10-13 represent the isothermal kinetic model. Each model requires staying at a constant pressure of 150 bar, or a constant temperature of 140ºC respectively.

We analyzed each rate constant for primary and secondary reactions, aiding in reactor performance simulation across various conditions of temperature, pressure, and reactor volume. These constants allowed for accurate predictions of the DMC production effort through simulations for the CSTR.

By integrating these kinetic formulas into our reactor design, we could simulate interactions between reactants and assess how DMC production responded to adjustments in temperature, as well as reactant and product levels. This step was vital for transitioning the process from laboratory to pilot scale, providing essential data for CIA's financial assessments regarding the new DMC production facility.

D - Level 1-5 Decisions and Mole Balances

Mole Balance Decisions

The primary objective is to establish the fundamental conceptual design of the process. This includes critical evaluations regarding the process's overall viability and the selection of a method for implementation. Our choice to employ a catalytic slurry based CSTR for DMC production is a pivotal Level 1 decision. This selection is based on a comprehensive review of historical data, economic viability, and the ready availability of CO_2 as a feedstock.

Reaction Decisions

Our decisions are centered on detailing the chemical processes and the stoichiometric balances of the key reactions producing DMC from CO_2. This stage involves selecting the basic reaction mechanisms, identifying the optimal conditions for achieving targeted yields, and ensuring the ethylene produced meets required purity standards. Our analysis at this level incorporates kinetic data and thermodynamic principles to understand how these reactions operate efficiently under specific conditions.

Recycle Decisions

The focus shifts to the process's optimization through the integration of recycle streams, aiming to enhance efficiency and maximize the use of resources. A significant assumption made at this stage is the complete recycling of the main reactants back into the reactor, which informs our strategy for managing byproducts and unused feedstocks. Design efforts at this level aim to increase DMC yield and minimize waste.

Separation Decisions

Our conceptual design begins the inclusion of energy balances across the plant for the in depth separation system. This considers both outsourced energy for reactor and separation demands.. The main assumption with this is that no heat is being lost to the surroundings wherever there is an introduction of energy or heat transfer. The objective of this level of design is to specify the direction of separation equipment and optimize on sizing and capex/opex for the separation equipment

Heat Integration Decisions

Our design aims to consider an overall energy balanced over the plant for streams. This becomes a question of heat exchanger integration and optimal heat transfer across the plant. We assume that heat losses from equipment and fouling is negligible at this point and focus on the ideal cases of heat exchangers and stream energy duty.

Mole Balance

Equations

$$s = 1 \tag{1}$$

$$r_2 = k_2 F_{EO} - k_1 r_{DMC} C E_V \tag{2}$$

$$r_3 = k_3 C E_V \tag{3}$$

$$\frac{C_{CO2}}{CE_0} = 13 \tag{4}$$

$$\frac{L_{ME0}}{CE_0} = 15 \tag{5}$$

EC:

$$F_{EC} - R_{EC} + CE_0 q - r_2 V - r_3 V = 0 \tag{6}$$

$$CE_{0,0} - CE_G + CE_0 q + CE_0 q - r_2 V - r_3 V = 0 \tag{7}$$

$$2 * EC_{0,0} - CE_0 - r_2 T - r_3 T = 0 \tag{8}$$

CO_2:

$$F_{CO2} - R_{CO2} + r_3 V - F_{EO} x = 0 \tag{9}$$

$$q CO_{2,0} - q CO_2 + r_3 V - EO_{0,0} = 0 \tag{10}$$

$$CO_{2,0} - CO_2 + r_3 T - EO_0 = 13 CE_0 - CO_2 + r_3 T - EO_{0,0} = 0 \tag{11}$$

MeOH:

$$F_{MeOH} - R_{MeOH} - 2 r_2 V - r_3 V = 0 \tag{12}$$

$$q MeOH_0 - q MeOH - 2 r_2 V - r_3 V = 0 \tag{13}$$

$$MeOH_0 - MeOH - 2 r_2 T - r_3 T = 15 CE_0 - MeOH - 2 r_2 T - r_3 T \tag{14}$$

$$P_{ME} = P_{DMC}(1 - \frac{s}{s}) \tag{1}$$

$$jP_{DMC} = P_{EG} = 3.3 \tag{2}$$

$$E_{EO} = \frac{P_{DMC}}{5} \tag{3}$$

$$iF_{MeOH} = 2P_{DMC} + P_{DMC}\left(1 - \frac{s}{s}\right) \tag{4}$$

$$jF_{CO2} = P_{DMC} \tag{5}$$

Level 3:

$$F_{CO2} = R_{CO2} + F_{CO2} \tag{6}$$

$$F_{MeOH} = R_{MeOH} + F_{MeOH} \tag{7}$$

$$13\frac{P_{DMC}}{s} = R_{CO2} + F_{CO2} \tag{8}$$

$$15\frac{P_{DMC}}{s} = R_{MeOH} + 2P_{DMC} + P_{DMC}\left(1 - \frac{s}{s}\right) \tag{9}$$

$$R_{MeOH} = 15\frac{P_{DMC}}{s} - 2P_{DMC} - P_{DMC}\left(1 - \frac{s}{s}\right) \tag{10}$$

Reactor:

$$EO : \text{ In - Out + Gen - Cons} = 0 \text{ (SS)} \tag{11}$$

$$\frac{E_{EO}}{q_{flow}} = \frac{P_{DMC}}{s} \tag{12}$$

$$q = \frac{F_A + F_B + \ldots}{q_A + q_B} \qquad (1)$$

$$\frac{REC}{F_{EC}} = q_{flow} - \frac{q_{EC}}{F_{EC}} = 0 \qquad (2)$$

$$\frac{q_{flow}}{F_{EC}} = \sum_{flow} q_{flow} \qquad (3)$$

$$q = \frac{F_{PROD}}{F_{PROD}} \qquad (4)$$

$$\sum_{F_{PROD}} = q\left(1 + \frac{\sum q}{q_{flow}}\right) \qquad (5)$$

E - Equipment Design Summary and HYSYS Process Flow Diagram

E.1 - Continuously Stirred Tank Reactor (CSTR) Design

CSTR calculations are based on the assumptions that mixing is complete and uniform throughout the tank, there is no distribution of residence times throughout the tank, and that the concentration of anyflow that enters the tank immediately becomes the concentration of the outlet stream. This allows us to derive algebraic equations to model the performance of a CSTR as follows:

$$\frac{F_{AO} - F_A}{V} = -r_A$$

Equation E.1.1

where F_A is the molar flow rate of species A, V is the volume of the reactor, F_{AO} is the initial flow of species A into the reactor, and r_A is the rate of reaction per unit volume for species A. For isothermal reactor conditions, the temperature dependency of the rate can be omitted.

The installed cost of the CSTR can be estimated from the reactor volume and material of construction:

$$Installed\ Cost\ (\$) = \left(\frac{M\&S}{280}\right) * 101.9 * D^{1.066} * H^{0.82} * \left(2.18 + F_c\right)$$

$$Where,\ F_c = F_m F_p$$

Equation E.1.2

Where M&S is the Marshall and Swift equivalent to 1800 for the year of 2024, D is the diameter of the CSTR, H is the height of the CSTR, F_m is the material correction factor (2.25 for our case

of a stainless steel cladCSTR), and F_p is the pressure correction factor (which is 2.5 due to operating pressure being at 150 bar)

E.2 - Separator / Splitter Design (W_{min})

The separation system design is intended for reactor effluent to be divided into recycle streams, product streams, and waste streams. For the scope of this preliminary design, the entire separation system is considered as one black box that has outlet streams that split our desired products perfectly. For our system we have four outlet streams from our separators that give a stream for product DMC, by product EG, recycled components of methanol, and waste streams of unused species. The perfect splitting gives each of these streams a composition of exclusively what is desired for them ie: recycled stream has only recycled components and no impurity.

The streams of our separation system are defined as follows: F_1 is DMC, F_2 is EG, F_3 is the recycle mix, and F_4 is the waste stream.

The following equation is how we analyzed the costing of our black box separation system including PSA:

$$W_{min} = \sum_i F_i RT_i (\sum_j x_j^i ln(\frac{x_j^i}{z_j}))$$

$$OPEX(\$/annum) = \lambda \bullet \epsilon W_{min}$$

Equation E.2.1

$$CAPEX(\$) = C_{en}(\lambda \bullet W_{min})$$

Equation E.2.2

Where, the summation over i is each different flow and the summation over j is each different species.. Additionally, λ is a correction factor which considers normal efficiencies for separation systems, and ϵ is the cost of energy in \$/GJ. These values are 35 and 3\$/GJ respectively for our case.

The capital expense of the separation system is given in Equation E.2.2 where C_{en} is the cost of energy in \$/W and is equivalent to 0.75 \$/W.

E.3 - Heat exchanger design

For each of the heat exchangers across the plant, including the reboilers and condensers of the distillation columns that will be discussed after this, were designed along what required Ua

would be needed to promote heat transfer at a maximum temperature along the equipment of 120°C. This cost correlation for the heat exchangers is as follows:

$$Installed\ Cost\ (\$) = \left(\frac{M\&S}{280}\right)\left(101.\ 3\ *\ A^{0.65}\ *\ F_c\right)$$

$$Where,\ F_c = \left(F_d + F_p\right)F_m$$

Equation E.3.1

Here A corresponds to the contact area between the hot and cold fluid of the respective heat exchanger. For our 2 heat exchangers, they have a contact area of: 3400 ft² and 3000 ft². F_d is the style of heat exchanger cost parameter, F_p is the pressure rating parameter, and F_m is the material choice parameter. All heat exchangers used were U-tube with stainless steel shells and tubes but had pressure ratings of 1 bar for both Thus giving cost parameters of: 0.85, 3.75, and 0-0.55 for F_d, F_m, and F_p respectively. This heat exchanger costing was used for both the stream heat exchanger and the jacketed cooler for the CSTR.

E.4 - Distillation tower design

Our design on distillation towers was based on the Underwood equation considering the relative volatilities of the main components that are expected in each tower. From this we determined an "ideal" reflux ratio, boil up ratio, and a minimum stages for each distillation tower. From these we systematically varied the calculated values to derive a more optimized cost for the equipment and have a lower energy cost. The costing of distillation towers is a combination of the pressure vessel costing, for the tower shell, heat exchanger costings, for the reboiler and condenser, and tray costing, for the trays inside. The installation cost for these towers is as follows:

Pressure vessel costing:

The costing of the pressure vessel is exactly the same as the equation used for the CSTR pressure vessel, however the F_p parameter changes to account for the operating pressure of each column.

Heat exchanger costing:

The costing of the heat exchangers were done by using equation E.3.1 and the same costing parameters with the only change being in the operating pressure where we rated them to operate up to 25 bar.

Tray costing:

Trays were costed under the assumption that we were using sieve trays with 24 inch spacing and tray material of stainless steel. The installed cost is shown below.

$$Installed\ Cost\ (\$) = \left(\frac{M\&S}{280}\right)\left(4.\ 7\ *\ D^{1.55}\ *\ H\ *\ F_c\right)$$

$$Where,\ F_c = F_s + F_t + F_m$$

In this equation, D is the diameter of the trays in feet, H is the height of the stacked trays of the total column, and each of the F parameters correspond to the spacing, tray type, and material of the trays, each of which are 1 for 24in tray spacing, 0 for sieve trays, and 1.7 for stainless steel respectively.

F - Economic Assumptions, Formulas, and Spreadsheets

For capital expenses we have an ISBL, OSBL and Contingency which sum up to be our total fixed capital cost (TFCC). For the inside battery limit(ISBL) we made the assumption that only the installation costs for our equipment would be considered within the scope of this preliminary design since it gives a very strong estimate for the largest costs that are directly integrated into our chemical plant. For the OSBL, we make the assumption that it is equivalent to 40% of the ISBL due to generalized cost estimates[14]. Contingency, which is our safety and predicted accident money that is set aside, is estimated to be 25% of the sum of ISBL and OSBL. We assume that at year 0, 1 and 2 we spend 25% of the TFCC in each of these years and then spend the last 25% in year 3 along with the entire WC (which is defined as 2 months worth of feedstock for full plant production).

The salvage cost of our plant is given as 5% of the TFCC and therefore is taken as a negative cash flow at the end of our plant life (12 years after plant start up) and is added to revenue for the last year in our cash flow.

Our revenue is determined to be the money made from selling DMC and the byproduct stream of Ethylene Glycol. As well, our AGS (money towards administration and operators) is given as 5% of our revenue and must then be taken away from profit as a cost of manufacturing. The cost of manufacturing(COM) also includes the feedstock price of CO_2, methanol, and ethylene oxide, the carbon sequestration price, the natural gas price, and AGS. The difference between revenue and COM is taken as our gross profit.

We determine a taxable income per year by subtracting depreciation of equipment from our gross profit. This depreciation is assumed to be 10 year linear for all equipment bought and the percentage of tax relief is given as:

$$D_i = \frac{cost\ basis}{equipment\ life}$$

$$cost\ basis\ =\ 1.1 * (2.28\ +\ ISBL)$$

Equation F.1

From this taxable income, we introduce the tax rate over our plant which is 27% to determine how much we pay in taxes and determine a cash flow using the following equation:

$$Cash\ flow\ =\ (REV\ -\ COM) * (1 - t) + D$$

Equation F.2

Where, cash flow is a per year, non discounted, after tax value for how much money our process generates. REV is the yearly revenue of our plant, COM is the cost of manufacturing, t is the tax rate, and D is depreciation each year. The present value (PV) is the cash flow at each year divided by the discount factor at each year. The equation is as follows:

$$PV = \frac{Cash\ Flow}{(1+enterprise\ rate)^n}$$

Equation F.3

Where, enterprise rate is the given value of 15% and n is the year in which each cash flow is from.

This gives a dollar amount of present value of any specific year. This is then used to determine a net present value (NPV) which is calculated as the sum of all previous PVs up to the year that an NPV is calculated at. The equation is as follows:

$$NPV_j = \sum_i^j PV_i$$

Equation F.4

Where, j is the year at which NPV is calculated for, and i is 0 to consider all present values from year 0 onward.

This value of NPV gives a good estimate of whether or not our design will produce positive investment results as dollar values equated to today's dollars even though the profit will come later. This is the most important calculation for the preliminary design and is paramount to deciding whether or not to go forward with the project and eventually benign construction of the chemical plant.

CashFlow Diagram
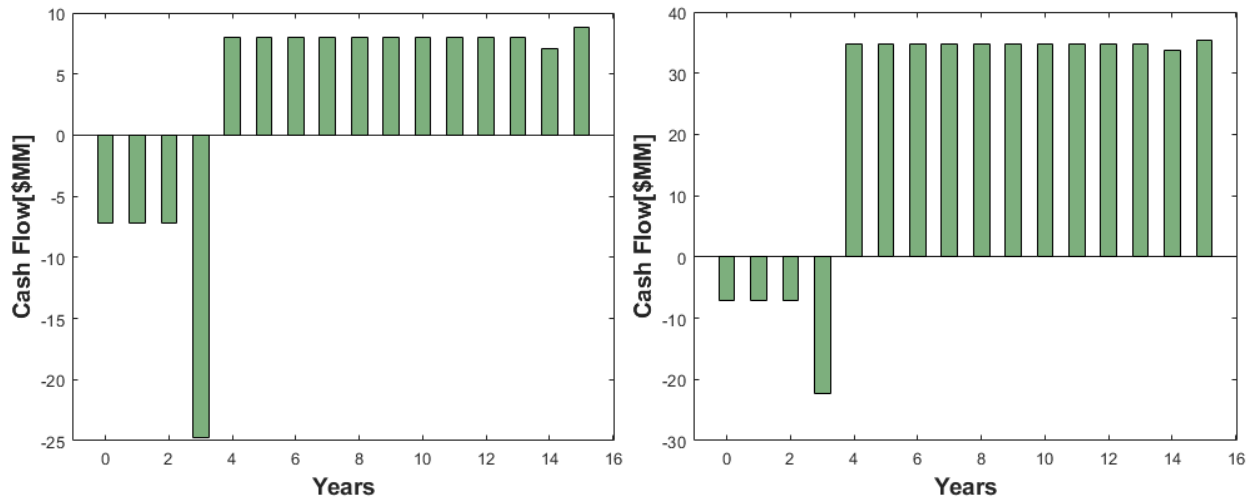
Figure F.1: Comparison of cash flows for the base case species prices and the european real market species values. Base case is the figure on the left and the European market values is shown on the figure to the right

Economic SpreadSheet

CIA
123 Lagoon Road
Santa Barbara, CA

ECONOMIC ANALYSIS

Economic Analysis With Given Species Sale Value								
Rev	Date	BY	APVD	Rev	Date	BY	APVD	
V1.1		EKT						

Plant Location
Case Description

REVENUES AND PRODUCTION COSTS		CAPITAL COSTS		CONSTRUCTION SCHEDULE					
	$MM/yr		$MM	Year	% FC	% WC	% SU	% FCOP	% VCOP
Main product revenue	110.0	ISBL Capital Cost	12.7	0	25%				
Byproduct revenue	34.1	OSBL Capital Cost	5.1	1	25%				
Raw materials cost	105.1	Indirect Cost	6.7	2	25%				
Utilities cost	14.4	Contingency	4.4	3	25%	100%	100%		
Consumables cost	0.0	Total Fixed Capital Cost	28.9	4				100%	100%
CO_2 sustainability charge	9.3			5				100%	100%
VCOP	94.7	Working Capital	17.5	6+				100%	100%
Salary and overheads	0.0	Start-up Costs	0.0						
Maintenance	0.0	Land	0.0						
Interest	0.0	Total Capital Investment	46.4						
AGS	5.5								
FCOP	5.5								

ECONOMIC ASSUMPTIONS

On Stream	8400 hr/yr	Discount Rate	15%	Depreciation method	Straight-Line	
	350 day/yr	Tax Rate	27%	Depreciation period	10 yrs	
Project Life	15 yr	Salvage Value	5%	Cost Basis	31.83363 $MM	

CASH FLOW ANALYSIS

All figures in $MM unless indicated

Project Year	Cap. Ex.	Revenue	COM	Gr. Profit	Deprcn.	Taxable Inc	Taxes Paid	Cash Flow	PV of CF	NPV	IRR	NV
0	7.2	0.0	0.0	0.0	0.0	0.0	0.0	-7.2	-7.2	-7.2	#NUM!	-7.2
1	7.2	0.0	0.0	0.0	0.0	0.0	0.0	-7.2	-6.3	-13.5	#NUM!	-14.4
2	7.2	0.0	0.0	0.0	0.0	0.0	0.0	-7.2	-5.5	-19.0	#NUM!	-21.7
3	24.7	0.0	0.0	0.0	0.0	0.0	0.0	-24.7	-16.3	-35.2	#NUM!	-46.4
4	0.0	110.0	100.2	9.8	3.2	6.6	1.8	8.0	4.6	-30.7	#NUM!	-38.4
5	0.0	110.0	100.2	9.8	3.2	6.6	1.8	8.0	4.0	-26.7	#NUM!	-30.4
6	0.0	110.0	100.2	9.8	3.2	6.6	1.8	8.0	3.5	-23.2	-21%	-22.4
7	0.0	110.0	100.2	9.8	3.2	6.6	1.8	8.0	3.0	-20.2	-10%	-14.4
8	0.0	110.0	100.2	9.8	3.2	6.6	1.8	8.0	2.6	-17.6	-4%	-6.5
9	0.0	110.0	100.2	9.8	3.2	6.6	1.8	8.0	2.3	-15.3	1%	1.5
10	0.0	110.0	100.2	9.8	3.2	6.6	1.8	8.0	2.0	-13.4	4%	9.5
11	0.0	110.0	100.2	9.8	3.2	6.6	1.8	8.0	1.7	-11.7	6%	17.5
12	0.0	110.0	100.2	9.8	3.2	6.6	1.8	8.0	1.5	-10.2	8%	25.5
13	0.0	110.0	100.2	9.8	3.2	6.6	1.8	8.0	1.3	-8.9	9%	33.5
14	0.0	110.0	100.2	9.8	0.0	9.8	2.6	7.1	1.0	-7.9	10%	40.6
15	0.0	112.3	100.2	12.1	0.0	12.1	3.3	8.8	1.1	-6.8	11%	49.4

ECONOMIC ANALYSIS

NPV	15 years	-6.8 $MM	Total Project IRR	11%	
NPV at yr	15	-6.8 $MM			

NOTES

1. All cash flows are assumed to occur at the end of the project year.
2.
3.

Figure F.2.1: Economic overall flow sheet considering given market prices

CIA
123 Lagoon Road
Santa Barbara, CA

ECONOMIC ANALYSIS

Economic Analysis With European Real Market Species Values									
	Rev	Date	BY	APVD	Rev	Date	BY	APVD	
	V1.1		EKT						

Plant Location
Case Description

REVENUES AND PRODUCTION COSTS

	$MM/yr
Main product revenue	100.2
Byproduct revenue	66.1
Raw materials cost	91.2
Utilities cost	14.4
Consumables cost	0.0
CO_2 sustainability charge	9.3
VCOP	48.8
Salary and overheads	0.0
Maintenance	0.0
Interest	0.0
AGS	5.0
FCOP	5.0

CAPITAL COSTS

	$MM
ISBL Capital Cost	12.7
OSBL Capital Cost	5.1
Indirect Cost	6.7
Contingency	4.4
Total Fixed Capital Cost	28.9
Working Capital	15.2
Start-up Costs	0.0
Land	0.0
Total Capital Investment	44.1

CONSTRUCTION SCHEDULE

Year	% FC	% WC	% SU	% FCOP	% VCOP
0	25%				
1	25%				
2	25%				
3	25%	100%	100%		
4				100%	100%
5				100%	100%
6+				100%	100%

ECONOMIC ASSUMPTIONS

On Stream	8400 hr/yr	Discount Rate	15%	Depreciation method	Straight-Line	
	350 day/yr	Tax Rate	27%	Depreciation period	10 yrs	
Project Life	18 yr	Salvage Value	5%	Cost Basis	31.83363 $MM	

CASH FLOW ANALYSIS

All figures in $MM unless indicated

Project Year	Cap. Ex.	Revenue	COM	Gr. Profit	Deprcn.	Taxable Inc	Taxes Paid	Cash Flow	PV of CF	NPV	IRR	NV
0	7.2	0.0	0.0	0.0	0.0	0.0	0.0	-7.2	-7.2	-7.2	#NUM!	-7.2
1	7.2	0.0	0.0	0.0	0.0	0.0	0.0	-7.2	-6.3	-13.5	#NUM!	-14.4
2	7.2	0.0	0.0	0.0	0.0	0.0	0.0	-7.2	-5.5	-19.0	#NUM!	-21.7
3	22.4	0.0	0.0	0.0	0.0	0.0	0.0	-22.4	-14.7	-33.7	#NUM!	-44.1
4	0.0	100.2	53.8	46.3	3.2	43.1	11.6	34.7	19.8	-13.9	-12%	-9.4
5	0.0	100.2	53.8	46.3	3.2	43.1	11.6	34.7	17.2	3.4	19%	25.3
6	0.0	100.2	53.8	46.3	3.2	43.1	11.6	34.7	15.0	18.4	32%	60.0
7	0.0	100.2	53.8	46.3	3.2	43.1	11.6	34.7	13.0	31.4	39%	94.6
8	0.0	100.2	53.8	46.3	3.2	43.1	11.6	34.7	11.3	42.7	42%	129.3
9	0.0	100.2	53.8	46.3	3.2	43.1	11.6	34.7	9.9	52.6	44%	164.0
10	0.0	100.2	53.8	46.3	3.2	43.1	11.6	34.7	8.6	61.2	46%	198.7
11	0.0	100.2	53.8	46.3	3.2	43.1	11.6	34.7	7.5	68.6	46%	233.3
12	0.0	100.2	53.8	46.3	3.2	43.1	11.6	34.7	6.5	75.1	47%	268.0
13	0.0	100.2	53.8	46.3	3.2	43.1	11.6	34.7	5.6	80.7	47%	302.7
14	0.0	100.2	53.8	46.3	0.0	46.3	12.5	33.8	4.8	85.5	48%	336.5
15	0.0	102.4	53.8	48.5	0.0	48.5	13.1	35.4	4.4	89.9	48%	371.9

ECONOMIC ANALYSIS

NPV	15 years	89.9 $MM	Total Project IRR	48%	
NPV at yr	15	89.9 $MM			

NOTES

1. All cash flows are assumed to occur at the end of the project year.
2.
3.

Figure F.2.2: Economic overall flow sheet considering the European real market values for species

HYSYS process flow diagram
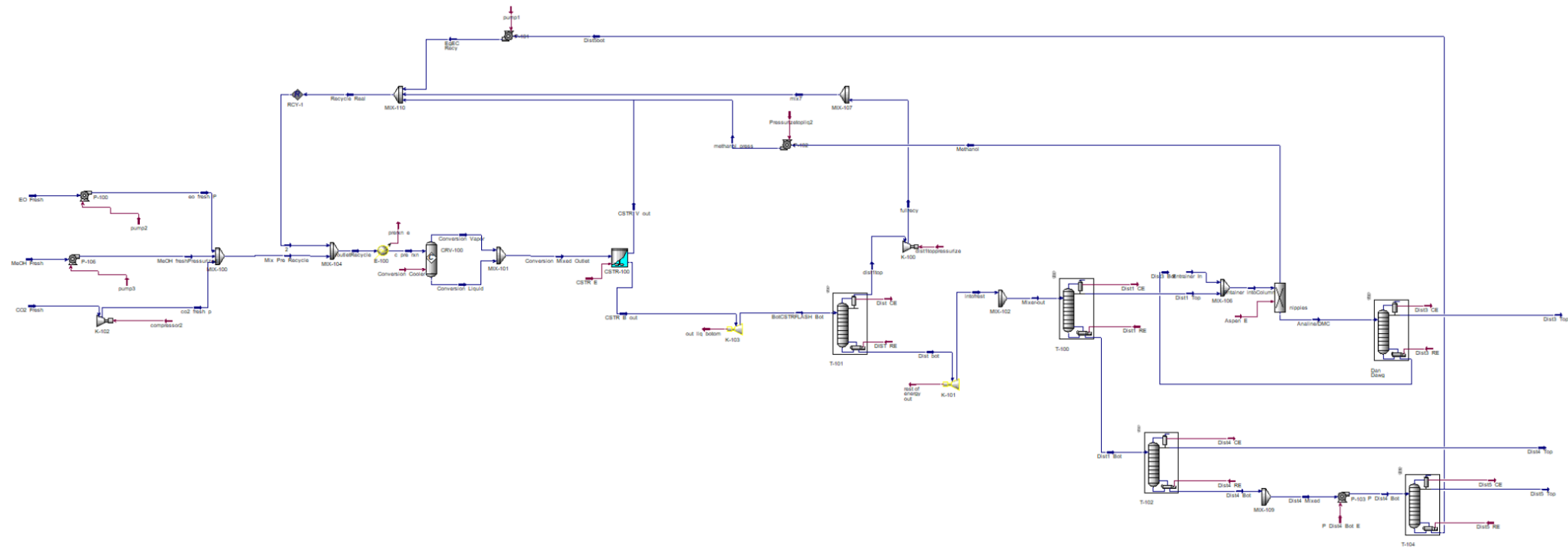
G - Considerations of Global, Cultural, Social, Environmental, and Economic Factors Related to This Project

Global Factors

The global demand for dimethyl carbonate (DMC) is on the rise, driven by its diverse applications as a green solvent, in battery electrolytes, and as a key intermediate in polycarbonate production. This surge in demand is notable in the rapidly expanding electric vehicle (EV) and electronics industries. Supporting this trend are international regulations that promote sustainable and environmentally friendly chemical processes, encouraging the use of CO_2 as a feedstock in DMC production. These policies aim to reduce carbon footprints and greenhouse gas emissions, fostering the adoption of CO2 utilization technologies. However, international trade policies, including tariffs and trade agreements, can impact the supply chain and market access for raw materials and finished products.

Cultural and Social Factors

Public perception of the chemical production industry is increasingly shaped by its environmental and social impact. The use of CO_2 as a feedstock in dimethyl carbonate production aligns with societal preferences for sustainable and green industrial processes, bolstering the plant's public image and community acceptance. It's crucial for the plant's operations to consider the social impact on the local community, including job creation, health and safety measures, and potential changes to the local environment. Engaging positively with the community and supporting local initiatives can further enhance social acceptance.

Environmental Factors

Using CO2 as a raw material in dimethyl carbonate production significantly reduces the plant's carbon contributions to a negative footprint. This environmentally friendly approach mitigates the impacts associated with traditional DMC production methods. These measures not only lower operational costs but also minimize emissions

Economic Factors

The economic viability of the dimethyl carbonate production plant hinges on several key factors, including the cost of raw materials such as CO_2, methanol, and catalysts, as well as energy, labor, and maintenance expenses. Optimizing these costs is crucial for maintaining profitability. Market prices for DMC fluctuate based on supply and demand dynamics. Securing investment and funding is vital for the plant's establishment, expansion, and technological upgrades. Attracting investors requires demonstrating the economic feasibility and sustainability of the plant. Government incentives, such as tax breaks, subsidies, and grants for using CO_2 in chemical production, can significantly enhance the plant's financial performance. These incentives promote the adoption of green technologies and sustainable practices, providing a competitive edge in the market to the older incumbent processes.

H - HAZOP and Safety Data Sheet

Hazop

Item	Parameter	Guide	Cause	Consequence	Safeguards	Recommendation
	Temperature	More	Heater Overperformance	Overheating of reactor contents	Thermal degradation of reactants/products, potential runaway reaction	Temperature control system, high-temperature alarms
		Less	Heater Underperformance	Inadequate heating	Incomplete reactions, accumulation of unreacted feed, low conversion rates	Backup heaters, low-temperature alarms
	Pressure	More	Blockage or Reaction Byproduct Buildup	Overpressure within the reactor	Leaks, equipment rupture, potential release of hazardous materials	Pressure relief valves, regular pressure monitoring

CSTR		Less	Inlet/Outlet Valve Malfunction	Low pressure within the reactor	Poor reactant flow, affecting reaction rates, potential vacuum condition	Vacuum breakers, pressure alarms
	Flow	More	Valve Failure Open	Excessive flow through the reactor	Increased reaction rates, potential for runaway reactions, overpressure	Flow meters, automatic control valves
		Less	Valve Failure Closed	Reduced flow through the reactor	Low reactant concentrations, poor conversion rates, potential overheating due to lack of cooling effect	Redundant flow paths, flow alarms
	Feed Flow	More	Valve Stuck	Increased flow to one side can cause high pressure, leading to	Flow monitoring	Install automatic shutdown systems

			Open	pipe rupture or equipment failure.	systems	for high flow conditions.
		Less	Valve Stuck Closed	Inadequate flow can cause low pressure, leading to poor separation efficiency and process downtime.	Pressure transmitters and alarms	Implement a fail-open control valve to maintain minimum flow.
	Temperature	More	Heater Control Failure	Overheating can cause fluid expansion and high pressure, risking leaks and material degradation.	Temperature control systems	Regular maintenance and inspection of heating elements.
Splitter		Less	Heater Control Failure	Too low temperature may increase viscosity, leading to incomplete separation and increased energy costs.	Temperature sensors with alarms	Use a redundant heating system to maintain optimal temperature.
	Pressure	More	Control Valve Failure	High pressure may exceed equipment design limits, leading to equipment failure or hazardous release.	Pressure relief valves	Conduct regular pressure relief system tests and inspections.
		Less	Inlet Blockage	Low pressure may cause poor separation and system inefficiencies.	Pressure indicators and alarms	Install a bypass line around the splitter for pressure maintenance.
	Composition	Off -spec	Feed Contamin- ation	Inconsistent product quality, could lead to downstream process impacts.	Online composition analyzers	Implement upstream purification steps and regular feedstock quality checks.

		Off-spec	Incorrect Feed Ratio	Suboptimal separation leading to waste of resources and energy.	Regular calibration of flow meters	Use precision control valves and flow meters for accurate feed ratio.
	Temperature	More	Control Failure	Overheating of the stream, potential for thermal degradation of fluids or materials, risk of fire or explosion.	High-temperature alarms, automatic shutdown systems.	Regularly test and maintain temperature control systems, install redundant temperature sensors.
		Less	Control Failure	Underheating of the stream, leading to inadequate process temperatures, possible solidification or increased viscosity of fluids.	Low-temperature alarms, backup heaters.	Implement procedures for heater switch-over in case of failure, ensure proper thermal insulation.
Heater	Flow Rate	More	Valve Stuck Open	Increased flow through heater, potential overheating or hot spots, energy wastage.	Flow control systems, overheat protection systems.	Install flow regulation valves, conduct routine checks on flow meters and control valves.
		Less	Valve Stuck Closed	Reduced flow through heater, poor heat transfer, process inefficiency.	Flow indicators, low-flow alarms.	Use fail-open valves, maintain a bypass line for alternative flow paths in case of valve failure.
	Pressure	More	Over	Potential for leaks, pipe rupture,	Pressure relief valves, burst	Regular inspection of pressure relief

			pressure	or heater damage.	disks.	devices, pressure monitoring.
		Less	InletOutlet Blockage	Inefficient heating, increased strain on heater components.	Pressure gauges, alarms.	Ensure routine maintenance and cleaning to prevent blockages.
Power Supply	Irregular		Power Surge/Fail	Unstable temperatures can lead to process interruption or equipment damage.	Surge protectors, UPS systems.	Install protective devices against surges, maintain backup power supply for critical heater operations.
	Loss		Power Outage	Complete process halt, risk of solidification or cold spots in the system.	Emergency power systems, alarms.	Regularly test backup power systems, ensure quick restoration of power or shutdown procedures.
Speed	More		Control Failure	Over-mixing can lead to shear damage to product, excessive energy consumption, or equipment wear.	Speed control systems, vibration detection systems.	Implement regular maintenance checks on mixer speed controls, install automated shutdown on vibration detection.
	Less		Control Failure	Under-mixing can result in an inhomogeneous product, affecting quality and downstream processes.	Speed sensors, torque monitoring.	Schedule periodic calibration of speed controls, ensure redundancy in sensing

						equipment.
Mixer	Temperature	More	Heating System Failure	Increased temperature can cause degradation of heat-sensitive materials, off-spec products.	Temperature control systems, thermocouples.	Regular inspection and testing of mixer heating elements, install temperature alarms.
		Less	Heating System Failure	Low temperature may not be sufficient for the reaction of the mixing process, resulting in poor quality.	Temperature gauges, low-temperature alarms.	Utilize a backup heating system, ensure proper thermal insulation.
	Pressure	More	Overfill or Gas Evolution	High pressure can cause seals to fail or create a hazardous environment, possible equipment damage.	Pressure relief devices, monitoring systems.	Conduct regular checks on pressure relief valves, install fail-safe shutdown systems.
		Less	Leak or Inadequate Sealing	Low pressure can result in ingress of contaminants or atmosphere, potentially compromising product quality.	Pressure sensors, leak detection systems.	Ensure regular inspection of seals and gaskets, maintain an inert atmosphere if required.
	Composition	Off-spec	Incorrect Proportion	Inaccurate mixing ratios can lead to an off-spec product, affecting subsequent processes and product quality.	Automated dosing systems, inline composition analysis.	Implement stringent quality control measures, regular calibration of dosing equipment.
		Contaminati	Cross contamina	Introduction of foreign materials can result in product spoilage or reactions creating hazardous	Regular cleaning schedules,	Schedule regular mixer cleaning, enforce strict

		on	tion	by-products.	contaminant monitoring.	contamination control protocols.
PSA	Adsorption Pressure	More	Control Valve Failure	High pressure can lead to bed compaction and desorbent losses, potential safety risks from vessel rupture.	Pressure relief valves, safety interlocks.	Install multiple independent pressure relief systems and frequent testing of control valves.
		Less	Leak or Valve Malfuncti-on	Low pressure can cause poor adsorption efficiency, leading to off-spec product and process inefficiency.	Pressure sensors, automatic leak detection.	Conduct regular system integrity checks and maintain a backup control valve.
	Desorption Pressure	More	Regenerat-ion Control Malfuncti-on	Excessive pressure during desorption can lead to desorbent waste and safety risks.	Pressure control systems, alarms.	Regularly calibrate and test pressure controllers, and have emergency shutdown procedures in place.
		Less	Improper Regenerat-ion Sequence	Inadequate desorption pressure can result in incomplete regeneration, reduced capacity for the next cycle.	System sequence checks, process timers.	Verify sequence operation regularly and ensure proper staff training on system operation.
	Time	More	Controller Failure	Extended cycle time can reduce throughput and increase wear on valves and adsorbents.	Cycle timers, flow monitors.	Implement strict maintenance schedules for cycle controllers and related

					equipment.
	Less	Controller Failure	Reduced cycle time may not allow complete adsorption or desorption, leading to diminished separation performance.	System checks, performance monitoring.	Regularly review system performance data to ensure optimal cycle timing.
Temperature	More	Heater Failure	High temperatures can cause thermal degradation of the adsorbent material, safety risks.	Temperature sensors, cooling systems.	Monitor temperatures closely, maintain backup cooling capabilities.
	Less	Heater Failure	Low temperatures may lead to poor adsorbate release or increased energy use for regeneration.	Temperature alarms, redundant heaters.	Inspect and maintain heaters, ensure proper insulation to retain heat.
Composition	Off-spec	Feed Contamin-ation	Incorrect feed composition can lead to poor adsorption selectivity, reduced product purity.	Composition monitors, pre-treatment systems.	Implement upstream purification steps, conduct regular feedstock quality checks.
	Varied	Feed Variability	Variation in feed composition can result in fluctuating performance and product quality.	Inline analyzers, control systems adjustments.	Install advanced control systems to adjust process parameters dynamically.
Temperature	Less	Excessive cooling	Fluid solidification, possible blockages	Temperature alarms,	Regular calibration and

					automated controls	maintenance of temperature control systems
			capacity			
		More	Inadequate cooling	Product degradation, failure to meet process specifications	Backup cooling units, low-temp alarms	Evaluate cooling capacity and redundancy in system design
Cooler	Flow	More	Valve stuck open	Mechanical stress, premature equipment wear	Flow meters, automatic shutoff valves	Implement scheduled maintenance and inspections of flow systems
		Less	Valve stuck closed	Reduced cooling effectiveness, potential for overheating	Redundant flow paths, flow alarms	Design system with parallel cooling paths for reliability
	Pressure	More	Blockage or overfilling	Potential for rupture or leaks	Pressure relief valves, routine monitoring	Regular checks for blockages and pressure regulation adherence

		Less	Wear and tear, valve malfunction	Inefficient cooling, reduced system effectiveness	Pressure boosters, alarms	Routine inspections and maintenance of pressure components
Heat Exchanger	Temperature	More	Control system malfunction	Overheating leading to thermal expansion and stress	High-temp alarms, automatic shutoff	Regular testing and maintenance of temperature control systems
		Less	Insufficient heat transfer	Poor process performance, energy inefficiency	Low-temp alarms, auxiliary heaters	Regular performance evaluations and system audits
	Flow	More	Control valve failure open	Increased pressure and flow, leading to mechanical failure	Flow controllers, safety valves	Frequent calibration and maintenance of flow control valves
		Less	Control valve failure closed	Reduced heat transfer efficiency, potential system overheating	Backup flow paths, alarms	Install redundant flow systems for critical operations

	Pressure	More	System overpressure	Equipment stress, possible leaks or ruptures	Pressure relief systems, burst discs	Routine pressure relief system testing and personnel training
		Less	General wear or malfunction	Low pressure leading to inadequate thermal transfer	Pressure indicators, supplementary systems	Periodic checks and maintenance of pressure support systems
	Temperature	More	Heater malfunction	Degradation of products, potential for column damage	High-temp alarms, cooling systems	Monitor and maintain temperature controls, train operators
		Less	Insufficient heating	Ineffective separation, higher operating costs	Low-temp alarms, additional heaters	Evaluate heating capabilities and incorporate redundancy
Distillation Tower	Pressure	More	Excess pressure build-up	Risk of column failure and hazardous material release	Pressure relief valves, safety interlocks	Regular safety valve checks and emergency response training

		Less	Vacuum due to condenser failure	Poor vapor-liquid equilibrium affecting separation efficiency	Vacuum breakers, alarms	Maintain and inspect vacuum prevention devices regularly
	Flow	More	High internal reflux	Flooding of the column, reduced separation efficiency	Flow meters, control valves	Dynamic control of flow rates based on real-time data
		Less	Low internal reflux	Reduced throughput and potential column drying out	Minimum flow controls, flow indicators	Regular flow system checks to ensure continuous operation
	Temperature	More	Heater control failure	Overheating can lead to fluid degradation	Temperature sensors, high-temperature alarms	Regular inspection and testing of temperature control systems
		Less	Insufficient heating	Incomplete vaporization, affecting tower operation	Low-temperature alarms, backup heaters	Ensure adequate heating capacity and system redundancy
Kettle Reboile	Pressure	More	Valve failure or	Overpressure can lead to equipment rupture	Pressure relief valves,	Install multiple pressure relief

r			blockage		monitoring systems	devices and routine inspections
		Less	General wear and tear	Underpressure can cause poor heat transfer	Pressure sensors, alarms	Regular maintenance and checks of pressure components
	Level	More	Feed excess or control failure	Risk of overflow and safety hazards	Level indicators, overflow alarms	Implement automatic level control and regular checks
		Less	Inadequate feed	Low level can expose heating elements and damage them	Low-level alarms, feed control systems	Monitor feed rates and maintain minimum level requirements
	Temperature	More	Cooling failure	Overheating leading to system failure	Temperature alarms, automatic shutoff	Regular inspection and maintenance of cooling systems
		Less	Excessive cooling	Condensate may freeze, blocking flow	Low-temperature alarms, heaters	Monitor cooling rates, install temperature

						regulation
Conden ser	Pressure	More	Overpress ure from blockage	Potential for leaks or condenser rupture	Pressure relief valves, burst disks	Frequent checks and maintenance of pressure relief systems
		Less	Vacuum condition	Air ingress, affecting condensation efficiency	Vacuum breakers, pressure alarms	Ensure integrity of vacuum seals and routine checks
	Flow	More	Valve stuck open	Increased flow can overload the condenser	Flow meters, automatic control valves	Regular calibration of flow control systems
		Less	Valve failure closed	Reduced cooling efficiency	Redundant flow paths, flow alarms	Install parallel pathways for critical operations
	Flow	More	Impeller wear or misalignm ent	Excessive flow can cause system stress	Flow meters, control valves	Regular inspection and maintenance of impeller and alignment
		Less	Valve	Reduced flow leading to process	Backup	Implement routine

Pump	Pressure	More	Discharge blockage	Overpressure can damage pump and piping	Pressure relief valves, sensors	Regular checks of discharge lines and relief settings
			failure or clogging	inefficiency	pumps, flow alarms	cleaning and maintenance schedules
		Less	Suction pressure drop	Cavitation, leading to mechanical failure	Pressure gauges, low-pressure alarms	Monitor suction conditions and adjust as necessary
	Temperature	More	Overloading or friction	Overheating can lead to seal failure	Temperature sensors, cooling systems	Ensure proper lubrication and cooling of pump system
		Less	Ambient conditions	Low temperatures may cause fluid viscosity increase	Heaters, temperature monitoring	Preheat fluids in cold conditions to maintain viscosity
	Flow	More	Control failure	Excessive speeds can cause mechanical failure	Speed controls, vibration sensors	Regular monitoring and maintenance of speed control

						systems
		Less	Inlet blockage	Reduced output and efficiency	Inlet filters, alarms	Regular inspection and cleaning of inlet pathways
Expander	Pressure	More	Upstream pressure increase	Potential for overloading and damage	Pressure relief devices, monitors	Install and maintain upstream pressure regulation
		Less	Leakage or valve failure	Decreased performance, energy loss	Leak detection systems, seals	Routine checks for leaks and integrity of valves
	Temperature	More	Compression heat	Overheating can degrade components	Cooling systems, temperature sensors	Implement cooling measures and monitor temperature closely
		Less	Ambient temperature drop	Material contraction, mechanical issues	Thermal insulation, heaters	Use heaters and insulation to manage temperature effectively

Safety Data Sheet

Species	Flammability	Explosive Limits (v/v)	Toxicology	Corrosiveness
Ethylene Oxide (EO)	Extremely flammable gas (Category 1)	Lower: 3.0%, Upper: 100%	Toxic by inhalation, may cause cancer, mutagenic, irritant	Corrosive
Carbon Dioxide (CO_2)	Non-flammable gas	Not applicable	Can cause asphyxiation in high concentrations	Non-corrosive
Ethylene Carbonate (EC)	Non-flammable liquid	Not applicable	May cause eye and skin irritation, harmful if swallowed	Non-corrosive
Methanol (MeOH)	Highly flammable liquid (Category 2)	Lower: 6.0%, Upper: 36.5%	Toxic if inhaled, ingested, or absorbed through skin, may cause blindness	Non-corrosive
Dimethyl Carbonate (DMC)	Flammable liquid (Category 3)	Lower: 3.0%, Upper: 13.9%	May cause eye and skin irritation, harmful if swallowed	Non-corrosive
Ethylene Glycol (EG)	Non-flammable liquid	Not applicable	Harmful if swallowed, may cause kidney damage	Non-corrosive

I - Code

CSTR all plots code
```
clc;
clear;
close all;
tau = 5000;
P = 50;
F = getFlows_Isothermal(P,tau);  % whatever the function handle is
%                                         F                              =
[P_DMC,P_EG,P_ME,F_MeOH,F_EO,F_CO2,S,X_EC,VPlant,check,qPlant,R_EC,R_MeOH
,R_CO2];
P_DMC = F(:,1);
P_EG = F(:,2);
P_ME = F(:,3);
F_MeOH = F(:,4);
F_EO = F(:,5);
F_CO2 = F(:,6);
S = F(:, 7);
X_EC = F(:,8);
VPlant = F(:,9);
check = F(:,10);
qPlant = F(:,11);
R_EC = F(:,12);
R_MeOH = F(:,13);
R_CO2 = F(:,14);

flow_rxtr = F_MeOH + F_EO + F_CO2 + R_EC + R_MeOH + R_CO2;

flow_sep = R_EC + R_MeOH + R_CO2 + P_DMC + P_EG + P_ME;

molfrac_sep = zeros(5000,6);

molfrac_sep(:,1) = R_EC/flow_sep;
molfrac_sep(:,2) = R_MeOH/flow_sep;
molfrac_sep(:,3) = R_CO2/flow_sep;
molfrac_sep(:,4) = P_DMC/flow_sep;
molfrac_sep(:,5) = P_EG/flow_sep;
molfrac_sep(:,6) = P_ME/flow_sep;

figure(1) % selectivity as func of conv
plot(X_EC,S,'r','LineWidth',1.5)
xlabel('Conversion of EC')
```

```matlab
ylabel('Selectivity')

figure(2) % rxtr vol vs conv
semilogy(X_EC,VPlant/1000,'LineWidth',1.5)
xlabel('Conversion of EC','FontSize', 14, 'FontWeight','bold')
ylabel('Reactor Volume [m^3]', 'FontSize', 14, 'FontWeight','bold')

figure(3) % fresh feed flow of raw mat vs conv
plot(X_EC, F_MeOH, 'g',X_EC, F_EO, 'r',X_EC, F_CO2, 'b','LineWidth',1.5)
xlabel('Conversion of EC','FontSize', 14, 'FontWeight','bold')
ylabel('Fresh feed Flows [mol/s]','FontSize', 14, 'FontWeight','bold')
legend('MeOH', 'EO', 'CO_2', location='best')

figure(4) % prod flows vs conv
plot(X_EC, P_DMC, 'g', X_EC, P_EG, 'r', X_EC, P_ME, 'b','LineWidth',1.5)
xlabel('Conversion of EC','FontSize', 14, 'FontWeight','bold')
ylabel('Product Flows []','FontSize', 14, 'FontWeight','bold')
legend('DMC', 'Ethylene Glycol', '2-Methoxy', location='best')

figure(5) % recyc flow vs conv
plot(X_EC, R_EC,'r', X_EC, R_MeOH, 'b', X_EC, R_CO2, 'g', 'LineWidth',1.5)
xlabel('Conversion of EC','FontSize', 14, 'FontWeight','bold')
ylabel('Recycle Flows []','FontSize', 14, 'FontWeight','bold')
legend('EC', 'MeOH', 'CO_2', location='best')

figure(6) % total flow to rxtr vs conv
plot(X_EC, flow_rxtr, 'b', 'LineWidth', 1.5)
xlabel('Conversion of EC','FontSize', 14, 'FontWeight','bold')
ylabel('Flow to reactor []','FontSize', 14, 'FontWeight','bold')

figure(7) % total flow to the sep sys vs conv
plot(X_EC, flow_sep, 'b', 'LineWidth', 1.5)
xlabel('Conversion of EC','FontSize', 14, 'FontWeight','bold')
ylabel('Flow to separations []','FontSize', 14, 'FontWeight','bold')

figure(8) % mol frac of each comp to sep sys vs conv
plot(X_EC, molfrac_sep(:,1), 'r',X_EC, molfrac_sep(:,2), 'b', X_EC, molfrac_sep(:,3), 'g',
X_EC, molfrac_sep(:,4), 'c', X_EC, molfrac_sep(:,5), 'm', X_EC, molfrac_sep(:,6), 'k',
'LineWidth',1.5)
xlabel('Coversion of EC', 'FontSize', 14, 'FontWeight','bold')
ylabel('Mole fracs to separations')
```

NPV calculation code

```matlab
%give a V, T, Ptot to get a FA_sol...from this FA_sol, optimize NPV with it
```

```matlab
clc; clear; close all;
R = 8.3145;
P = 50;  %
% T = 120;
MnS = 1800;
%% Species Flows
tau = 3000;
F = getFlows_Isothermal(P,tau);  % what ever the function handle is
%                                F                                =
[P_DMC,P_EG,P_ME,F_MeOH,F_EO,F_CO2,S,X_EC,VPlant,check,qPlant,R_EC,R_MeOH
,R_CO2];
P_DMC = 36.77; %36.2
P_EG = 36.3; % 27.75
P_ME = 0.4; % 1
F_MeOH = 71; %69.44
F_EO = 37; %36
F_CO2 = 37.22; % 37.22
S = F(:, 7);
X_EC = F(:,8);
VPlant = F(:,9);
check = F(:,10);
qPlant = F(:,11);
R_EC = 0;
R_MeOH = 375;
R_CO2 = 523;
%% reaction heats
dH1 = -6.1e4; %J/mol
dH2 = -5.4e4; %J/mol
dH3 = -5.5e4; %J/mol

%% Project statement prices
price_DMC = 1100; % $/MT
```

```matlab
price_EG = 500; % $/MT
price_EO = 1250; % $/MT
price_CO2_tax = 125; % $/MT
price_CO2_stock = 45; % $/MT
price_MeOH = 600; % $/MT
price_ME = 0; %per MT
```

%% Real Market Prices

```matlab
% price_DMC = 1000; % $/MT
% price_EG = 970; % $/MT
% price_EO = 1460; % $/MT
% price_CO2_tax = 125; % $/MT
% price_CO2_stock = -72.5 *1.09; % $/MT, this is where we're given credit value for buying
CO2
% price_MeOH = 337; % $/MT
```

%% Beginning of costing analysis

```matlab
elek_price = 0.06 / 3600000; % $/J
BTU_W = 3.41; % convert from J/s to BTU/hr
steam_price = 3.84; % this is in units of $ * C/GJ, therefore divide by delta T and multiply by
power in GW to get variable cost of steam
% delT = 120; % this will be the estimated average delta T between process steam entering
and leaving in reboilers
%for i = 1:length(VPlant) % input optimal iteration number into for loop to go a single time
once best NPV is found
  i= 909;
  %% CSTR reactor costing



  F_m_cstr = [1]; % material rating factor
  F_p_cstr = [1.35]; % pressure rating factor  consider 150 bar
  F_c_cstr = F_m_cstr .* F_p_cstr;
```

D_cstr = 3.28 * (4^(1/3)*(VPlant(i)/1000)^(1/3))/pi^(1/3); % converted into feet for costing

H_cstr = D_cstr;

cstr_capex = (MnS/280) * 101.9 * D_cstr^1.066 * H_cstr^0.82 *(2.18 + F_c_cstr);

Hrxn1 = dH1 * R_EC * X_EC(i)/(1 - X_EC(i)); % under assmuption that all EC reacts instantly in CSTR, EC_0 * V = mol/s of EC

Hrxn2 = dH2 * P_DMC;

Hrxn3 = dH3 * P_ME;

rxn_heat = abs(Hrxn1 + Hrxn2 + Hrxn3); % in units of Joules/s

rxn_heat = (4.3+2.7)*1e6;

%% furnace costing(NO FURNACES)

duty_furn = [0]; % in units of J/s

F_d_furn = [1]; % furnace design type factor

F_m_furn = [0.75]; % material design factor

F_p_furn = [0]; % pressure rating factor

F_c_furn = F_d_furn + F_m_furn + F_p_furn;

furn_capex = sum((MnS/280) * 5.52e3 * (BTU_W * duty_furn/1e6).^(0.85) .* (1.27 + F_c_furn)); % this should just be in $

furn_opex = sum(3.0247e7 * 3/1e9 * duty_furn); % this is in units of $/annum

%% Heat exchanger costing

duty_hexs = [6.225e6]; % in joules, to be converted to BTU in respective equations

F_d_hexs = [0.85]; % taken as a U-tube style for all of these heat exchnagers (doesnt include reboilers)

F_p_hexs = [0]; % each hex pressure rating

F_m_hexs = [3.75]; % SS/SS material factor for each heat exchanger

F_c_hexs = F_m_hexs .* (F_d_hexs + F_p_hexs);

U_hexs = [770]; % will be chosen specifcilly for each heat exchanger

Tlm_hexs = [85]; %

A_hexs = 10.7 * (duty_hexs*BTU_W) ./ (U_hexs .* Tlm_hexs); % area of each of the heat exchangers

hexs_capex = sum((MnS/280) * 101.3 * A_hexs.^0.65 .* (2.29 + F_c_hexs)); % all hex capex excluding reboilers

%% Cooler exchangers costing (just rxtr cooler) no dist cond opex or capex

F_d_coolers = 0.85 * ones(1,1); % taken as a U-tube style

F_p_coolers = [0]; % up to atmospheric pressure with water on the cooling side,

F_m_coolers = 0 * ones(1,length(F_d_coolers)); % SS/SS materail exchanger for all

F_c_coolers = F_m_coolers .* (F_d_coolers + F_p_coolers);

U_coolers = [800]; % taken as U for high pressure liquds on inside and cooling fluid on outside

Tlm_coolers = [30]; % average given value since reactor is kept at steady value and not "cooling" along exchanger

cooler_duties = [abs(rxn_heat)]; % in J/s

A_coolers = 10.7 * (cooler_duties)./(U_coolers .* Tlm_coolers);

coolers_capex = sum((MnS/280) * 101.3 * A_coolers.^0.65 .* (2.29 + F_c_coolers)); % cooling jacket for CSTR capex

cost_cool_water = 3; % $ / GJ

coolers_opex = sum(3.024e7 * cost_cool_water/1e9 * cooler_duties); % something to do with cooling water or something to maintain SS temp of reactor

%% Flash costing (THERE ARE NO FLASHES)

D_flash = 3.28 * [0, 0]; % diameter of the flashes, meters converted to feet

H_flash = 3.28 * [13.33, 5]; % height of the flashes

F_m_flash = [2.25, 2.25]; % material factor for the flashes, stainless steel for both

F_p_flash = [1, 1]; % pressure rating for flashes

F_c_flash = F_m_flash .* F_p_flash;

flash_capex = sum((MnS/280) * 101.9 * D_flash.^1.066 .* H_flash.^0.82 .* (2.18 + F_c_flash));

%% expander costing (we get electricty from this and sell it so we gain moneies)

expander_duty = [120.8e3, 1.083e6]; % this must be in joules/s

expander_opex = sum(3.024e+7 * elek_price .* expander_duty); % in units of [$/annum]

%% compressor costings, including pumps, uses electricicty for power

F_c_comp = ones(1,5); % make this be a vector to account for multiple pieces of equipment, each cell is a given number for design factor

comp_duties = [120.3e3, 11.66e3, 19.53e3, 101.5e3, 1.245e3]; % in units of J/s

bhp = comp_duties ./ 745.7; % this is a power in horsepower

comp_capex = sum((MnS/280) * 517.5 * (bhp).^0.82 .* (2.11 + F_c_comp(1)));

comp_opex = sum(3.024e+7 .* elek_price .* comp_duties); % in units of [$/annum]

%% Distillation costing

D_dist = 3.28 * 1.5 * ones(1,6); % diameter of the tower in feet

H_dist = [60, 60, 60, 50, 60, 60]; % height of the tower in feet   %% ONLY 6 TOWERS IN THIS DESIGN

F_m_dist = 2.25 * ones(1,length(H_dist)); % material factor for the dist tower

F_p_dist = ones(1,length(H_dist)); % pressure rating for towers

F_p_dist(1) = 1.35;

F_c_dist = F_m_dist .* F_p_dist;

dist_tower_capex = sum((MnS/280) * 101.9 * D_dist.^1.066 .* H_dist.^0.82 .* (2.18 + F_c_dist));

D_trays = 1.5 * 3.28 * ones(1, length(D_dist));

H_trays = 2 * ones(1,length(D_trays));

F_s_trays = ones(1,length(H_dist)); % tray spacing factor [inches]

F_t_trays = zeros(1,length(H_dist)); % tray type ie:seive

F_m_trays = 1.7 * ones(1,length(H_dist)); % material rating for trays

F_c_trays = F_s_trays + F_t_trays + F_m_trays;

trays_capex = sum((MnS/280) * 4.7 .* D_trays.^1.55 .* H_trays .* F_c_trays);

F_m_reb_dist = 3.75 * ones(1,length(H_dist)); % material choice factor

F_d_reb_dist = 1.35 * ones(1,length(H_dist)); % desgin type factor for reboilers, (likely kettle reboilers if phase change)

F_p_reb_dist = zeros(1,length(H_dist)); % pressure rating factor for reboilers

F_c_reb_dist = F_m_reb_dist .* (F_d_reb_dist + F_p_reb_dist);

duty_reb = [1.4e6, 6.5e6, 1.7e6, 30e6, 3.6e6, 6.4e6];

% this is the duties for each of the distillation reboilers in J/s

  U_reb = 820 * ones(1,length(duty_reb)); % respective heat transfer coeff for each reboiler

  Tlm_reb = 40 * ones(1,length(duty_reb)); % each reboilers' Tlm

  A_reb_dist = 10.7 * (duty_reb) ./ (U_reb .* Tlm_reb);

  reb_dist_capex = sum((MnS/280) * 101.3 * A_reb_dist.^0.65 .* (2.29 + F_c_reb_dist));

  % reb_dist_opex = sum(3.024e+7 * 3/(1e9 * delT) .* duty_reb); % will just be costed using process steam to reheat

  F_m_cond_dist = 3.75 * ones(1,length(H_dist)); % condensors material factor

  F_d_cond_dist = 0.85 * ones(1,length(H_dist)); % design type factor. (will likely be normal U-tube exchangers)

  F_p_cond_dist = zeros(1,length(H_dist)); % pressure rating factor for condensors

  F_c_cond_dist = F_m_cond_dist .* (F_d_cond_dist + F_p_cond_dist);

  duty_cond = [4.8e6, 1.39e7, 100e3, 27e6, 1.5e6, 5.1e6];

% this is the duties for each of the distillation condensors

  U_cond = 770 * ones(1,length(duty_cond)); % respective heat transfer coeff for each condensor

  Tlm_cond = 40 * ones(1,length(duty_cond)); % each condensors' Tlm

  A_cond_dist = 10.7 * (duty_cond) ./ (U_cond .* Tlm_cond);

  cond_dist_capex = sum((MnS/280) * 101.3 * A_cond_dist.^0.65 .* (2.29 + F_c_cond_dist));

  cond_dist_opex = sum(3.024e+7 * 3/1e9 .* duty_cond); % must consider potentially really cold coolant for this

  dist_sys_capex = dist_tower_capex + trays_capex + reb_dist_capex + cond_dist_capex;

  %% Sep Sys costing (W min sep first off)

  lambda = 0; % efficiency factor for sep, we used 35

  c. = 0.75; % $/watt value, we used 0.75

  eps = 3; % $ cost of energy $/GJ, we used 3

  R = 8.3145;

```matlab
Tsep = 273.15;

F0 = P_DMC + R_CO2 + R_MeOH + R_EC + P_ME + P_EG;

F1 = P_DMC; % main product stream

F2 = R_CO2 + R_MeOH + R_EC; % all recycles

F3 = P_ME; % waste product

F4 = P_EG; % by product with sale price

z_sep = [P_DMC, P_EG, P_ME, R_MeOH, R_CO2, R_EC]./F0;

x_sep_1 = P_DMC./F1;

x_sep_2 = [R_CO2,R_MeOH, R_EC]./F2;

x_sep_3 = P_ME./F3;

x_sep_4 =  P_EG./F4;


   W_min = F1 * R * Tsep * x_sep_1 * log(x_sep_1) + F2 * R * Tsep * sum(x_sep_2 .*
log(x_sep_2)) ...

       + F3 * R * Tsep * sum(x_sep_3 .* log(x_sep_3)) + F4 * R * Tsep * sum(x_sep_4 .*
log(x_sep_4)) ...

    - F0 * R * Tsep * sum(z_sep .* log(z_sep)); % this is in units of J/s

  sep_sys_capex = c. * lambda * W_min ; % this must be in units of $, $/watt * watt

   sep_sys_opex = eps * lambda * W_min; % this must be in units of $/annum, $/GJ *
1GJ/1e9J * J/s * 3.024e+7s/50 weeks * 50 weeks/1annum


%% Net Present Value calc



years = (0:15)';

entpz = 0.15;

tax_rate = 0.27;

dscn = (1 + entpz) .^ years;



   %ISBL = sep_sys_capex + coolers_capex + cstr_capex + flash_capex + dist_sys_capex +
comp_capex + hexs_capex + furn_capex; % + dist_sys_capex + comp_capex; % all equipment
costing capex
```

ISBL = cstr_capex + dist_sys_capex + comp_capex + coolers_capex; % + dist_sys_capex + comp_capex; % all equipment costing capex

OSBL = 0.4 * ISBL;   %more in depth would be to find amount of electricity used from outsource

contingency = (ISBL + OSBL) * 0.25;

TFCC = 1.3* (ISBL + OSBL + contingency);

salvage = 0.05;

elek_NRG = sum(comp_duties) - sum(expander_duty); % this is the total energy used via electricity in J/s, estimation could be around 15 MW

Steam_NRG = sum(duty_reb(1:5)); % total energy used by natrual gas in J/s, estimation could be around 40 MW

NG_NRG = sum(duty_reb); % NRG used as NG to heat this reboiler in J/s

NG_CO2_prod = 3.024e7 /891e3 * 44.01 * 1e-6 * NG_NRG; %MT of CO2 per year

elek_CO2_prod = (800 * 3.024e+7)/(1e6 * 3.6e6) * elek_NRG; % this should be in MT/annum ... $/annum = $/MT * MT/kg * lbsC02/kWhr * kg/lbs * J/s * s/annum

if elek_CO2_prod < 0

elek_CO2_prod = 0;

end

% NG_CO2_prod = (44.01 * 3.024e+7)/(885e3 * 1e6) * NG_NRG; % this should also give a value of MT/annum ... $/annum =

Purchased_CO2 = (F_CO2 * ((3.024e+7 * 44.01)/(1e6))); % tons of CO2 purchased per annum as feed...gives tax break as well

CO2_prod_tax = price_CO2_tax * (elek_CO2_prod + NG_CO2_prod); %[$/annum] but get CO2 tax break since we buy CO2

% CO2_prod_tax = 10000000;

EO_stock_cost = price_EO * F_EO * ((3.024e+7 * 44.052)/(1e6)) ; % cost of fresh sock feed in $/annum, US price is $1100/MT, $/MT * mol/s * s/annum * g/mol * MT/g

CO2_stock_cost = price_CO2_stock * Purchased_CO2; % cost of stock CO2 $/annum

MeOH_stock_cost = price_MeOH * F_MeOH * ((3.024e+7 * 32.04)/(1e6)); % more reasonable price is $350

% Ani_stock_cost =

Tot_stock_cost = EO_stock_cost + CO2_stock_cost + MeOH_stock_cost;

STEAM_cost = steam_price * 1e-9 * Steam_NRG * 3.024e7 ; % in $/annum

elek_cost_tot = elek_NRG * elek_price * 3.024e7; % this is in $/annum

Refrige_cost = cond_dist_opex + coolers_opex; % multiply each duty by its respective neccesary refridgerant cost.... $/kg * kg/kJ * power/time -> $/annum

NG_cost = 3.024e7 * 3 * 1e-9 * NG_NRG;

utilities = STEAM_cost + elek_cost_tot + Refrige_cost + NG_cost ; % $/annum

WC = 2/12 * (Tot_stock_cost); % 2 months of raw materials

capex = [1/4*TFCC ; 1/4*TFCC ; 1/4*TFCC ; 1/4*TFCC + WC ;0;0;0;0;0;0;0;0;0;0;0;0];

rev = price_DMC * P_DMC * ((3.024e+7 * 90.078)/(1e6)); % main product revenue for polymer grade DMC $/ton * ton/kilo ton * kilo ton/annum = $/annum

% rev = 110000000;

byprodrev = (price_EG * P_EG + P_ME * price_ME) * ((62.07 * 3.024e+7)/(1e6)) ; % by product revenue with EG, $/ton * ton/1e6g * 76.09g/mol * mol/s * 3.024e+7s/annum = $/annum

revenue = rev * [0;0;0;0;1;1;1;1;1;1;1;1;1;1;1;1];

REV = revenue; % revenue vector

AGS = 0.05 * REV; % gives just a vector for the payment to workers / administration

MAX_EV = rev + byprodrev - Tot_stock_cost;

% Heat_exchange_savings = 35e6; % estimated savings in $MM

```matlab
    VCOP = (CO2_prod_tax + Tot_stock_cost + utilities - byprodrev); %variable costs of
production with psa... essentially a OPEX
  FCOP = AGS(end); % fixed costs of production could consrder other


  COM = (VCOP + FCOP) * [0;0;0;0;1;1;1;1;1;1;1;1;1;1;1;1]; % energy costs and continuous
raw material costs


  GRprof = REV - COM;



  cost_basis = 1.1 * (2.28 * ISBL);


   depriciation = cost_basis * [0;0;0;0;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0.1;0;0]; %ten year
linear dpereiciation model



  tax_inc = GRprof - depriciation;
  for b = 1:16
    if tax_inc(b) < 0
      tax_inc(b) = 0;
    end
  end
  tax_paid = tax_rate * tax_inc;


  CashFlow = (REV(:) - COM - depriciation) .* (1 - tax_rate) - capex + depriciation;
  CashFlow(16,1) = CashFlow(16,1) - TFCC*salvage;
  PV = CashFlow./dscn;


  NPV = zeros(16,1);
  NV = zeros(16,1);


    for j = 2:length(years)
      NPV(1) = PV(1);
```

```
        NPV(j) = PV(j) + NPV(j-1);
    end




    for k = 1:length(years)
        NV(k) = sum(CashFlow,1:k);
    end




    CFD = table(years, capex, REV, COM, GRprof, depriciation, tax_inc, tax_paid, CashFlow,
PV, NPV, NV);


    Money(i) = CFD{16,"NPV"};




%end

x = Money(i);
y = i;
sprintf('Max NPV $MM:  %0.5g',x/1e6)
sprintf('Reactor Volume m^3 : %0.5g',VPlant(y)/1e3)
% npv(T) = x;
% % % plot(VPlant,Money)
% % % xlabel("Reactor Volume [L]")
% % % ylabel("NPV [$], 15yr, 15% dcr")
% % % ylim([0 2e8])
% % % figure(1)
% % %
% % %
```

```matlab
% % % flash_per = flash_capex/ISBL;
% % % dist_per = dist_sys_capex/ISBL;
% % % cstr_per = (cstr_capex)/ISBL;
% % % furn_per = furn_capex/ISBL;
% % % cooler_per = coolers_capex/ISBL;
% % % hexs_per = hexs_capex/ISBL;
% % % comp_per = comp_capex/ISBL;
% % %
figure(2)
X = [cstr_capex,dist_sys_capex,hexs_capex,comp_capex,coolers_capex];
Labels = {'{\bfCSTR}','{\bfDistillations}','{\bfHeat Exchangers}','{\bfCompressors}','{\bfCoolers}'};
xPercent = X / sum(X) * 100;
newLabels = [];
for i=1:length(X)
    newLabels = [newLabels {sprintf('%s (%.1f%%)', Labels{i}, xPercent(i))}];
end
pie(X, newLabels);
title('ISBL [$12.7MM]')


figure(3)
X = [CO2_prod_tax, utilities, AGS(end)];
Labels = {'{\bfCO2 Tax}','{\bfUtilities}','{\bfAGS}'};
xPercent = X / sum(X) * 100;
newLabels = [];
for i=1:length(X)
    newLabels = [newLabels {sprintf('%s (%.1f%%)', Labels{i}, xPercent(i))}];
end
pie(X, newLabels);
title('OPEX [$94.7MM/year]')
```

Sensitivity analysis and econ bar graphs

clc;clear;close all;

Variables = { 'Construction time [years]','ISBL [$MM]','Interest rate [%]','TFCC [$MM]','CO2 tax [$/MT]', ...
    'CO_2 feed price [$/MT]','EG value [$/MT]' ,'Raw Materials[$MM/year]','DMC price [$/MT]'};

UB_affect = [-63.8 47.6 11 -11.5 -9.20 -7.9 -8.9 -14 -11.6];

LB_affect = [50.2 -67.1 -24.5 -2.1 -3.70 -5.1 -4.7 9.4 -1.9];

Nominal_NPV = -6.8;

total = abs(-LB_affect + UB_affect);
[total,ind] = sort(total,'ascend');
LB_affect = LB_affect(ind);
UB_affect = UB_affect(ind);

figure()
a = barh(LB_affect,'FaceColor', [0.8500 0.3250 0.0980]); % Dark orange
hold on
b = barh(UB_affect,'FaceColor', [0.3010 0.7450 0.9330]); % Light blue
legend([a, b], {'Variable loss', 'Variable gain'}, 'Location', 'Southwest');
c = get(a,'BaseLine');
set(c,'BaseValue',Nominal_NPV);
set(gca,'yticklabel',Variables)
xtickformat('$%,.0f MM')
xlabel('NPV [$MM]', 'FontSize', 14, 'FontWeight','bold')

NPV1 = [-7.2 -13.5 -19.0 -35.2 -30.7 -26.7 -23.2 -20.2 -17.6 -15.3 -13.4 -11.7 -10.2 -8.9 -7.9 -6.8];

NPV2 = [-7.2 -13.5 -19.0 -33.7 -13.9 3.4 18.4 31.4 42.7 52.6 61.2 68.6 75.1 80.7 85.5 89.9];

CashFlow1 = [-7.2 -7.2 -7.2 -24.7 8.0 8.0 8.0 8.0 8.0 8.0 8.0 8.0 8.0 8.0 7.1 8.8];

CashFlow2 = [-7.2 -7.2 -7.2 -22.4 34.7 34.7 34.7 34.7 34.7 34.7 34.7 34.7 34.7 34.7 33.8 35.4];

years = 0:15;

barWidth = 0.5;

barSpacing = 0.1;

figure(2)

bar(years, NPV1, barWidth, 'FaceColor', [0.5 0.7 0.5]);

xlabel('Years', 'FontSize', 14, 'FontWeight','bold');

ylabel('NPV [$MM]', 'FontSize', 14, 'FontWeight','bold');

figure(3)

bar(years, NPV2, barWidth, 'FaceColor', [0.5 0.7 0.5]);

xlabel('Years', 'FontSize', 14, 'FontWeight','bold');

ylabel('NPV [$MM]', 'FontSize', 14, 'FontWeight','bold');

figure(4)

bar(years, CashFlow1, barWidth, 'FaceColor', [0.5 0.7 0.5]);

xlabel('Years', 'FontSize', 14, 'FontWeight','bold');

ylabel('Cash Flow[$MM]', 'FontSize', 14, 'FontWeight','bold');

figure(5)

bar(years, CashFlow2, barWidth, 'FaceColor', [0.5 0.7 0.5]);

xlabel('Years', 'FontSize', 14, 'FontWeight','bold');

ylabel('Cash Flow[$MM]', 'FontSize', 14, 'FontWeight','bold');

Isothermal CSTR function

```
% CSTR 507 Isothermal
function F = getFlows_Isothermal(P,tau)
%const
%T is const at 140C
% R = 8.3145;
CO2_P = readmatrix('CO2_P.xlsx');
rho_CO2_M = CO2_P(:,3)*1000; % g/L
%P_CO2_M = CO2_P(:,2); %bar

rho_CO2 = rho_CO2_M(P-49); %density of CO2 at correct index

MR_CO2_EC = 13;
MR_MeOH_EC = 15;

rho_MeOH = 0.792/32.04*1000;
rho_DMC = 1.07/90.08*1000;
rho_EC = 1.32/88.06*1000;
rho_ME = .965/76.09*1000;
rho_EG = 1.11/62.07*1000;

rho_CO2_m = 5.59;

if  rho_CO2 <= 246.82
   I_k2f = 0.013;
end
if rho_CO2 > 246.82
   I_k2f = 0.02486-4.943e-5*rho_CO2;
end
I_k2r = 0.01486*rho_CO2^(-0.873);
I_k3 = 3.014e-4*exp(-5.99e-3*rho_CO2);

C_EC_0 = 1/(1/rho_EC+MR_CO2_EC/rho_CO2_m+MR_MeOH_EC/rho_MeOH);
p = struct();
p.C_CO2_0 = MR_CO2_EC*C_EC_0;
p.C_MeOH_0 = MR_MeOH_EC*C_EC_0;
max_tau = tau;
X_EC = zeros(max_tau,1);
S = zeros(max_tau,1);
qPlant = zeros(max_tau,1);
VPlant = zeros(max_tau,1);
check = zeros(max_tau,1);
P_DMC = zeros(max_tau,1);
```

```matlab
P_EG = zeros(max_tau,1);
P_ME = zeros(max_tau,1);
F_MeOH = zeros(max_tau,1);
F_EO = zeros(max_tau,1);
F_CO2 = zeros(max_tau,1);
R_MeOH = zeros(max_tau,1);
R_EC = zeros(max_tau,1);
R_CO2 = zeros(max_tau,1);

options = optimset('Display','off');
p.k2f = I_k2f;
p.k2r = I_k2r;
p.k3 = I_k3;
p.C_EC_0 = C_EC_0;
i = 1;
for j = 1:max_tau
    tau = j;


    p.tau = tau;



    fun = @(x) paramfun(x,p);
    x0 = 1*ones(1,6);
    x = fsolve(fun, x0,options);
        check(i) = x(1)/rho_EC + x(2)/rho_DMC + x(3)/rho_EG + x(4)/rho_CO2_m +
x(5)/rho_MeOH + x(6)/rho_ME;
    C_EO_0 = C_EC_0-x(1);

    X_EC(i) = (C_EC_0-x(1))/(C_EC_0); % converted EC / inlet EC conc
    S(i) = x(2)/C_EO_0; % DMC / EO selectivity
    %P_DMC_mol_s = 100e6/50*1000/90.078/604800;
        % qPlant(i) = 2*P_DMC_mol_s/x(1) + P_DMC_mol_s/x(1)* (1-S(i))/S(i) +
2*P_DMC_mol_s/x(1) + P_DMC_mol_s/x(1)*((1-S(i))/S(i))...
    %   + P_DMC_mol_s/x(1); %DMC + EG (x2) + ME + MeOH +CO2 + 0*EO
    %
    % VPlant(i) = qPlant(i)*tau;
    P_DMC(i) = 100e6/50*1000/90.078/604800; % mol/s
    P_EG(i) = P_DMC(i);
    P_ME(i) = P_DMC(i) .* (1-S(i))./S(i);
    F_MeOH(i) = 2*P_DMC(i) + P_DMC(i).*((1-S(i))./S(i));
    F_EO(i) = P_DMC(i)./(S(i));
    F_CO2(i) = P_DMC(i);
        %qPlant(i) = P_DMC(i)/rho_DMC + P_EG(i)/rho_EG + F_CO2(i)/rho_CO2_m +
F_MeOH(i)/rho_MeOH + P_ME(i)/rho_ME;
```

```matlab
    %qPlant(i) = (P_DMC(i)/rho_DMC + P_EG(i)/rho_EG + F_CO2(i)/rho_CO2_m +
F_MeOH(i)/rho_MeOH + P_ME(i)/rho_ME)*rho_EC/(rho_EC-x(1));
        qPlant(i) = -(P_DMC(i)/rho_DMC + P_EG(i)/rho_EG + P_ME(i)/rho_ME)/(-1 +
x(1)/rho_EC+x(4)/rho_CO2_m+x(5)/rho_MeOH);
    R_EC(i) = x(1)*qPlant(i);
    R_CO2(i) = x(4)*qPlant(i);
    R_MeOH(i) = x(5)*qPlant(i);
    VPlant(i) = qPlant(i)*tau;
    i=i+1;
end

% P_DMC = 100e6/50*1000/90.078/604800*ones(length(VPlant),1); % mol/s
% P_EG = P_DMC;
% P_ME = P_DMC .* (1-S)./S;
% F_MeOH = 2*P_DMC +  P_DMC.*((1-S)./S);
% F_EO = P_DMC./S;
% F_CO2 = P_DMC;
F                                                                          =
[P_DMC,P_EG,P_ME,F_MeOH,F_EO,F_CO2,S,X_EC,VPlant,check,qPlant,R_EC,R_MeOH
,R_CO2];

  function conc = paramfun(C, p)
     C_EC = C(1);
     C_DMC = C(2);
     C_EG = C(3);
     C_CO2 = C(4);
     C_MeOH = C(5);
     C_ME = C(6);

     C_DMC_0 = 0; %assumes perf sep
     C_EG_0 = 0;  %assumes perf sep
     C_ME_0 =0;   %assumes perf sep
     k2f = p.k2f;
     k2r = p.k2r;
     k3 = p.k3;
     tauf = p.tau;
     C_EC_0f = p.C_EC_0;
     C_CO2_0 = p.C_CO2_0;
     C_MeOH_0 = p.C_MeOH_0;
     r2 = (k2f * C_EC^0.8 - k2r * C_DMC*C_EG);
     r3 = k3 * C_EC;

     conc = real([C_EC_0f - C_EC  - tauf*(r2+r3);
         C_CO2_0 - C_CO2 + r3*tauf;
         C_MeOH_0 - C_MeOH - 2*tauf*r2 - r3*tauf;
         C_DMC_0 - C_DMC + r2*tauf;
```

```
            C_EG_0 - C_EG + r2*tauf;
            C_ME_0 - C_ME + r3*tauf ]);

    end
end
```

Isobaric CSTR function
```
function F = getFlows_Isobaric(T,tau)
%vary T and set max tau ~ 1000 for large number of data points
%%
% F = [P_DMC,P_EG,P_ME,F_MeOH,F_EO,F_CO2,S,X_EC,VPlant] order of solutions
% returned
%%
T = T+ 273.15;
R =8.314;
MR_CO2_EC =13; %const

MR_MeOH_EC = 15; %const

P_k2f = 6.59e+2 * exp(-37200/(R*T));
P_k2r = 1.19e+4 * exp(-53700/(R*T));
P_k3 = 1.89e+6 * exp(-82400/(R*T));
% k2f = 6.59e+2 * exp(-37200/(R*T));
% k2r = 1.19e+4 * exp(-53700/(R*T));
% k3 = 1.89e+6 * exp(-82400/(R*T));
rho_EO = 0.882*1000/44.05;
%rho_CO2 = 0.771/44*1000;
rho_CO2 = 5.59;
rho_MeOH = 0.792/32.04*1000;
rho_DMC = 1.07/90.08*1000;
rho_EC = 1.32/88.06*1000;
rho_ME = .965/76.09*1000;
rho_EG = 1.11/62.07*1000;

C_EC_0 = 1/(1/rho_EC+MR_CO2_EC/rho_CO2+MR_MeOH_EC/rho_MeOH);

p = struct();
p.C_CO2_0 = MR_CO2_EC*C_EC_0;
p.C_MeOH_0 = MR_MeOH_EC*C_EC_0;

max_tau = tau;
X_EC = zeros(max_tau,1);
S = zeros(max_tau,1);
qPlant = zeros(max_tau,1);
```

```matlab
VPlant = zeros(max_tau,1);
check = zeros(max_tau,1);
P_DMC = zeros(max_tau,1);
P_EG = zeros(max_tau,1);
P_ME = zeros(max_tau,1);
F_MeOH = zeros(max_tau,1);
F_EO = zeros(max_tau,1);
F_CO2 = zeros(max_tau,1);
R_MeOH = zeros(max_tau,1);
R_EC = zeros(max_tau,1);
R_CO2 = zeros(max_tau,1);

options = optimset('Display','off');
i=1;
for j = 1:max_tau
tau = j;

p.k2f = P_k2f;
p.k2r = P_k2r;
p.k3 = P_k3;
p.tau = tau;
p.C_EC_0 = C_EC_0;

 fun = @(x) paramfun(x,p);
   x0 = 1*ones(1,6);
   x = fsolve(fun, x0,options);
   check(i) = x(1)/rho_EC + x(2)/rho_DMC + x(3)/rho_EG + x(4)/rho_CO2 + x(5)/rho_MeOH
+ x(6)/rho_ME;
   C_EO_0 = C_EC_0-x(1);

   X_EC(i) = (C_EC_0-x(1))/(C_EC_0); % converted EC / inlet EC conc
   S(i) = x(2)/C_EO_0;

X_EC(i) = (C_EC_0-x(1))/(C_EC_0); % converted EC / inlet EC conc
S(i) = x(2)/C_EO_0; % DMC / EO selectivity
   P_DMC(i) = 100e6/50*1000/90.078/604800; % mol/s
   P_EG(i) = P_DMC(i);
   P_ME(i) = P_DMC(i) .* (1-S(i))./S(i);
   F_MeOH(i) = 2*P_DMC(i) +  P_DMC(i).*((1-S(i))./S(i));
   F_EO(i) = P_DMC(i)./(S(i));
   F_CO2(i) = P_DMC(i);
       qPlant(i)  =  -(P_DMC(i)/rho_DMC  +  P_EG(i)/rho_EG  +  P_ME(i)/rho_ME)/(-1  +
x(1)/rho_EC+x(4)/rho_CO2+x(5)/rho_MeOH);
   VPlant(i) = qPlant(i)*tau;
   R_EC(i) = x(1)*qPlant(i);
   R_CO2(i) = x(4)*qPlant(i);
```

```matlab
    R_MeOH(i) = x(5)*qPlant(i);
    i=i+1;
end



F                                                                          =
[P_DMC,P_EG,P_ME,F_MeOH,F_EO,F_CO2,S,X_EC,VPlant,check,qPlant,R_EC,R_MeOH
,R_CO2];

% figure(1)
% plot(X_EC,S,'LineWidth',2,'Color','r')
%
% figure(2)
% plot(X_EC,check,'LineWidth',2,'Color','b')
%
% figure(3)
% semilogx(VPlant,P_DMC,VPlant,P_EG,VPlant,P_ME,...
%     VPlant,F_MeOH,VPlant,F_EO,VPlant,F_CO2)
% legend('P_DMC','P_EG','P_ME','F_MeOH','F_EO','F_CO2')
%
% figure(4)
% semilogy(X_EC,VPlant)

function conc = paramfun(C, p)
    C_EC = C(1);
    C_DMC = C(2);
    C_EG = C(3);
    C_CO2 = C(4);
    C_MeOH = C(5);
    C_ME = C(6);

    C_DMC_0 = 0; %assumes perf sep
    C_EG_0 = 0;  %assumes perf sep
    C_ME_0 =0;   %assumes perf sep
    k2f = p.k2f;
    k2r = p.k2r;
    k3 = p.k3;
    tauf = p.tau;
    C_EC_0f = p.C_EC_0;
    C_CO2_0 = p.C_CO2_0;
    C_MeOH_0 = p.C_MeOH_0;
    r2 = (k2f * C_EC^0.8 - k2r * C_DMC*C_EG);
    r3 = k3 * C_EC;

    conc = real([C_EC_0f - C_EC  - tauf*(r2+r3);
        C_CO2_0 - C_CO2 + r3*tauf;
```

```
                C_MeOH_0 - C_MeOH - 2*tauf*r2 - r3*tauf;
                C_DMC_0 - C_DMC + r2*tauf;
                C_EG_0 - C_EG + r2*tauf;
                C_ME_0 - C_ME + r3*tauf]);

    end
end
```

J - Team Member Work Statement

Team Member Work Statement

Name of team member here   George Weule

State here what you contributed to the design project and report

Appndix   Hysys
some writing   graphs

Name of team member here   Alan Stoev

State here what you contributed to the design project and report

Writing, MATLAB (PFR +
NPV optimization)

Name of team member here   Ethan

State here what you contributed to the design project and report

Writing, MATLAB (NPV,
Sensitivity, mol balance)
Economic flowsheets / CFDs

Print Name and Sign: _____ Date: 3/12

Print Name and Sign _____ Date: 3/12

Print Name and Sign _____ Date: 3/12

Rating of Team Members for Design Project

Please rate each group member's contributions in the categories below:
1-2 - unsatisfactory, 3 - acceptable/adequate, 4 – very good, 5 - excellent
Each member fills out one form and signs the bottom.

Name :	1) George	2) Alan	3) Ethn
Quality of work presented	5	5	5
Quantity of work performed	5	5	5
Effort	5	5	5
Punctuality (meetings and deadlines)	5	5	5
Knowledge of design methods	5	5	5
Class attendance	5	5	5

Communication 5   5   5

Do you feel that each member of the group deserves the same grade? If not, who does
not and why?

Yes

It's important to note that differences in performance will not necessarily affect
individual grades; however, large discrepancies may result in differences in grades.

Additional comments:

good team :)

Print Name and Sign: _____ Date: 3/12