Production of PolyMethylMethAcrylate (PMMA) through the Alpha Process

Oh No, Oh No, Oh No, Oh No, OEAA

Team Members:

Orry Nihangame

Elton Tsai

Alex Guo

Ahmad Elrefaie

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Rensselaer Polytechnic Institute

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Executive Summary

The OEAA group is proposing a scaled-up production of general purpose Polymethylmethacrylate (PMMA) in the form of beads to be sold to various end-user industries. The proposed plant design utilizes an industrially prevalent process commonly used in the production of PMMA known as the Alpha Process to produce at a plant capacity of 58,482 metric tonnes per year. The Alpha Process was chosen as the optimal process based on a number of factors. Primarily, the OEAA group considered feedstock accessibility/pricing, environmental, health and safety risks, and the technological feasibility of the process.

Additionally, the optimal location for the plant was decided based on a number of metrics including feedstock accessibility/price, regional growth rate, legislative regulations, and competition. Using the various determined metrics, the optimal plant location was decided to be in the Hefei economic and technological development zone, located in China's Anhui province. The area boasts a number of competitive advantages including, but not limited to, easy access to feedstock from nearby ethylene and methanol production facilities, cheap labor and capital costs, and most notably, minimal competition with respect to PMMA production in the area.

The global market's compound annual growth rate (CAGR) was determined to be an average of 7.32% ± 1.13%, with a total addressable market of 4.79 ± 0.13 billion dollars. Furthermore, the CAGR for the beads market in particular was found to be 9.1%, justifying the production of beads in place of other PMMA products. The Anhui province was selected as the prime location for a PMMA producing facility due to the fact that the Asia-Pacific region was unanimously found to be the fastest growing market for PMMA products.

The Alpha Process uses ethylene, methanol, and carbon monoxide as starting materials for the production of PMMA. The reactions are performed in conjunction with a metal catalyst intended to increase the yield and selectivity of methyl propionate, which is later separated from excess methanol and catalyst to be recycled and reused in the original reactions. The methyl propionate is then reacted with formaldehyde via the use of a fixed bed reactor to produce MMA monomer, which is then further polymerized into PMMA through free radical polymerization.

Risks on the production of PMMA as a final product vary in type; the three primary risks involved in the production of PMMA were determined to be safety, technical, and economic risks. The safety risks generally include the chemical, plant, and public safety, which can often be mitigated through the implementation of training routines, alarm systems, and process control measures that ensure the safety of all involved in the unlikely event that safety issues arise. Technical risks of noteworthy mention are the introduction of new materials that adequately replace PMMA due to lower cost and similar function as well as competing technologies with the Alpha Process. Mitigation of these risks can only be realistically done through cost minimization and ensuring that an optimal plant location is chosen; however, it is necessary to note that neither of these risks present a short term impact on PMMA production in Asia. Lastly, economic risks involve the fluctuation of feedstock availability. The effects of these risks are expected to be mitigated by the plant's location and its proximity to potential feedstock suppliers. After a thorough analysis of a proposed plant design, the OEAA team projects a cumulative cash flow of \$1.05 Bn and a net present value (NPV) of \$376.82 MM. Additionally, a feasibility analysis examining the potential for a price increase on the most volatile feedstock revealed that the plant remains reasonably profitable, even at significantly increased operating costs. Ultimately, the proposed complete plant design is determined to be feasible, and extremely profitable.

1. Introduction

1.1 Background

Polymethylmethacrylate (PMMA) is a transparent, thermoplastic polymer that is often used as a substitute for glass due to its high shatter-resistance, high light transmission, and high weather resistance[1]. Its diversity in properties and applications has led to its implementation in a number of different industries ranging from the simple production of sheets in the signs and displays industry (billboards) to use in the automobile industry (tail lights). In recent years, the

PMMA industry has been rapidly expanding due to the versatility of this material; as such, it has become a point of interest for the OEAA group as a potential target material to be mass-produced for sale to end-user industries. The market for PMMA is ever growing, and the processes by which it is processed are well-known at this point, making the decision to produce PMMA an informed, calculated decision with known risks and potential setbacks. Large volumes of PMMA imports suggest a potential need for new plants, especially in regions of high demand for PMMA. The decision to pursue the production of PMMA at a large scale is assessed by analyzing the global PMMA market for possible growth trends, and further analyzing regional markets to determine the most suitable target market. Further, the technological aspect of the production is considered by contrasting the various processes by which PMMA is made in industry. Based on these aspects, the ideal location and process for a plant is decided, and the risks associated with such decisions are assessed. These necessary precautions are taken to ensure the economic and technical feasibility of a PMMA production plant in the current market.

1.2 Market Assessment

1.2.1 End-User Industries of PMMA

The most highly demanding end-users of PMMA consist of producers of signs and displays, construction, automotive, electronics, and others (medical/dental applications)[3-5]. The signs and displays industry utilizes PMMA in the form of plastic sheets to produce durable billboards and other types of illuminated signs, while the construction industry uses it primarily in the form of extruded sheets for windows. The electronics industry employs PMMA for the production of phone screens and light guide panels (LGP) of LED devices[6]. Lastly, in the automotive industry, PMMA is used for car parts such as for the headlight lens/housing[7].

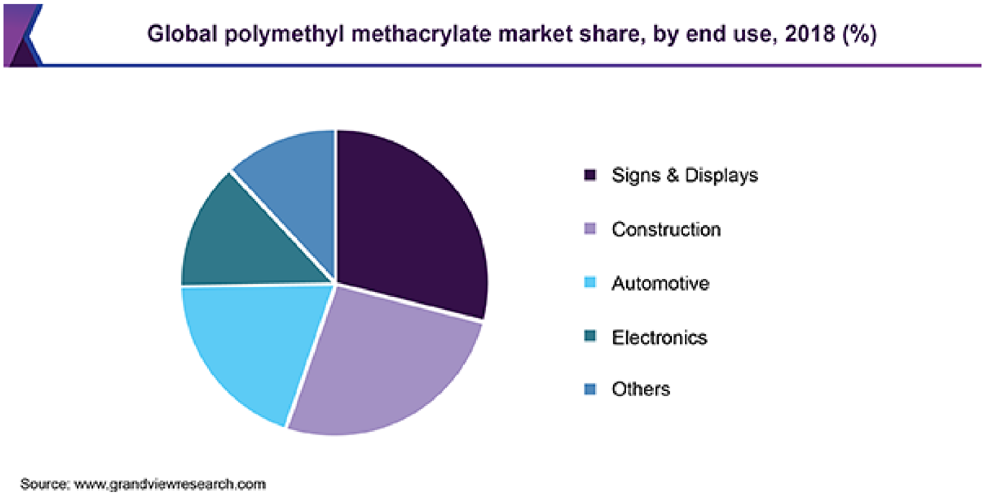


Figure 1: Distribution of End-User Industries for PMMA[4]

Figure 1 above shows that the market volumes of PMMA used in the various end-user industries vary only slightly from one to another, with signs and displays being the largest source of PMMA usage in the world.

1.2.2 Total Addressable Market (TAM) and Growth

Since its commercialization, PMMA has been ever expanding in its usage in several fields. As a result, global demand for PMMA has been sharply rising, which has reflected in the market's compound annual growth rate (CAGR). According to several market research groups, the CAGR for the PMMA market ranges from 6 to 9% globally. [4,9-13]

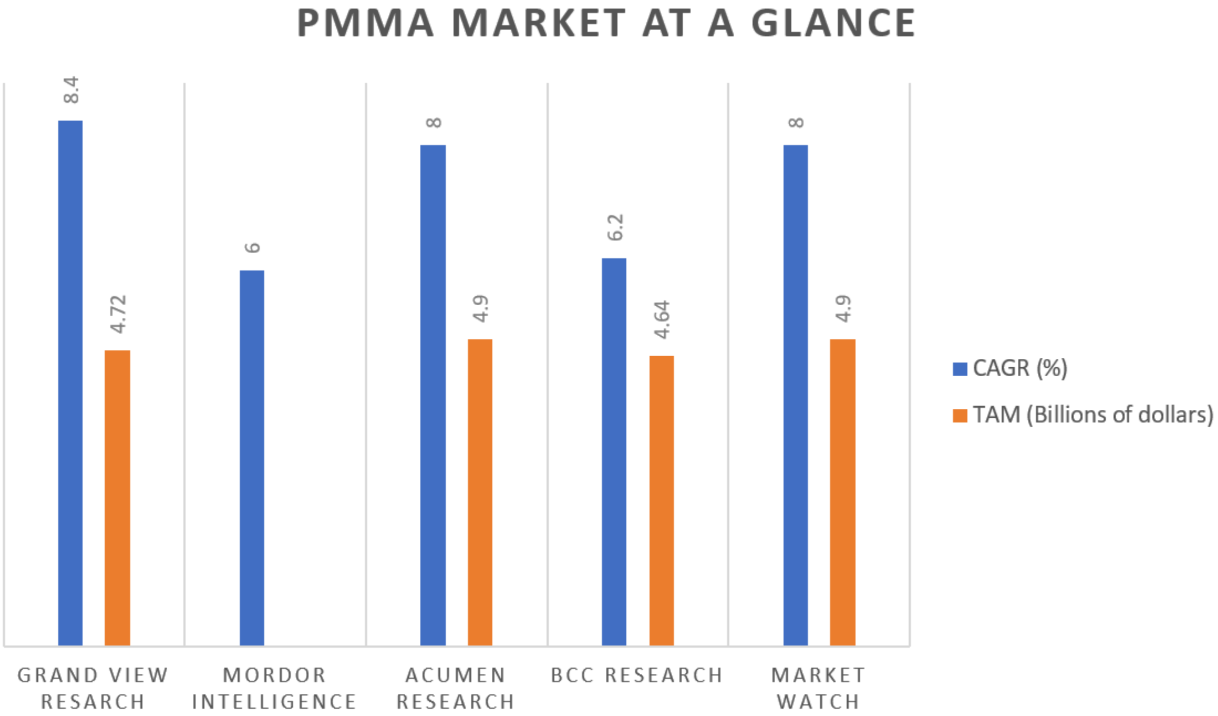


Figure 2: PMMA TAM and CAGR from several market reports[11]

The data gathered from the various sources used suggested an average CAGR of 7.32% ± 1.13%, and an average total addressable market of 4.79 ± 0.13 billion dollars. The five reports in Figure 2 suggest that the largest markets for PMMA exist primarily in the United States of America, Europe, and the Asia Pacific region.[4,9-13] Although the global market is characterized by an overall growth rate and market volume, all five utilized resources for the statistics unanimously agree that the largest growing markets are those within the Asia-Pacific region, making the countries in this region potentially worthwhile targets for a chemical plant focused on the production of PMMA.[4,9-13] A trend report produced by Evonik Corporation suggests that a little under two thirds of overall PMMA demand is sourced from Asia, with China being the main source of this demand.[18] Additionally, the source suggests that more than half of Chinese demand is met by importation. Meanwhile, 17% of global demand is due to countries residing in Europe, while another 14% is from North America.[19]

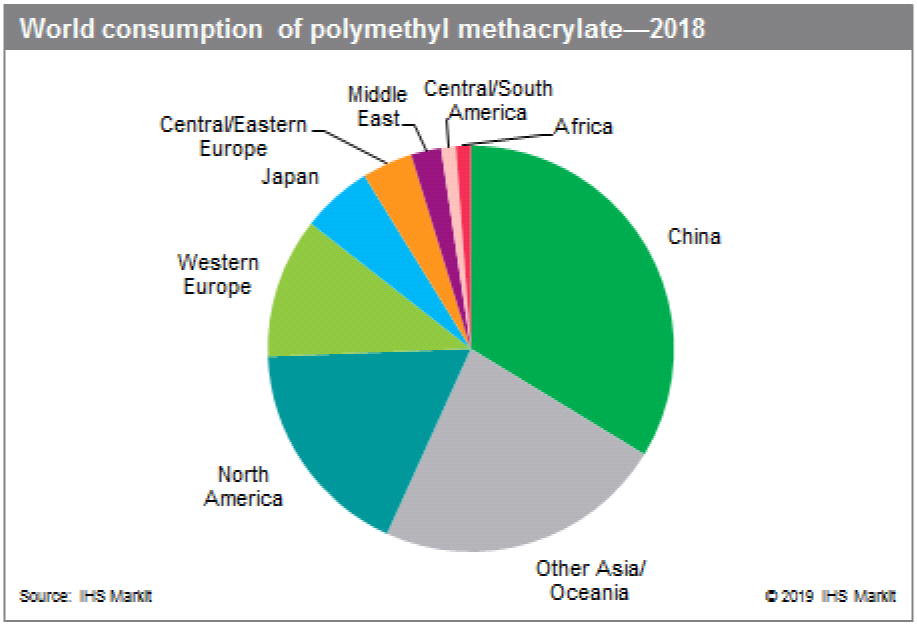


Figure 3: Global Market by Country[25]

Evidently, demand for PMMA is highest primarily in Asia with China, India, Taiwan, South Korea, and Japan being five of the top ten countries importing PMMA for local use.

Figure 4: Top 10 Countries importing PMMA (2016)[11]

Although these statistics are from 2016, many of these countries are still showing similar, consistent demand for PMMA.

Data sourced from Independent Commodity Intelligence Services (ICIS) presents the overall throughput of plants producing PMMA throughout the world suggesting an average capacity of approximately 33,500 tonnes per year[14] . The data include plants varying from a capacity of just 3000 tonnes per year to a maximum of 90,000 tonnes per year[14]. Selecting a target plant capacity is helpful in considering the serviceable obtainable market. By anticipating a serviceable obtainable market, OEAA hopes to meet the needs of the market without producing excess, as suggested by the green engineering principles listed by the American Chemical Society[16]. Further description of specific plant location and justification for location choice is described in Section 4.1.

1.2.3 Market Segmentation by Form

As mentioned before, the market for PMMA is primarily segmented into forms such as extruded sheets, beads, resins, and various other products, while the end-user segmentation for all these various types of material can be divided into the construction, automotive, electrical, and other industries[12].

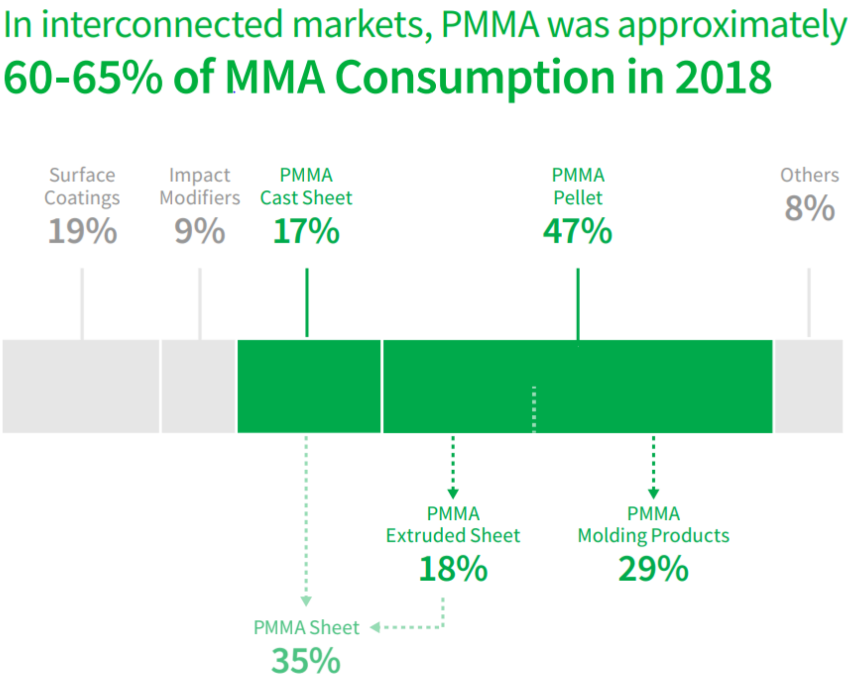


Figure 5: Segmentation by form (note that the Figure represents MMA market segmentation, not just PMMA segmentation)[8]

Keeping in mind the various options during PMMA production, it is important to analyze the needs of end-user industries. According to several market research groups, the fastest growing segment of PMMA production is bead production with an average CAGR of 9.1%, while the largest market volume for PMMA production is attributed to extruded sheets [4,13]. However, unlike sheets, beads have the most diversity with regards to end-user industry use. For example, they can often be used as a "texturing agent for thermoplastics or coatings," while they can also be further developed into extruded sheets should the need arise[4]. Additionally, beads can be processed into complex shapes using injection molding. An example of a molding product is a car headlight lens/housing. PMMA cast sheets account for about one-fourth of PMMA use by form and are produced with the cell cast process, where the polymerization and molding process occur concurrently. Although the PMMA cell cast process produces very high quality sheets as compared to extrusion of PMMA beads, it is more technically complicated and restricted in applications to end-user industries[2]. The large rate of growth in the bead market alongside its diversified use makes it a viable option for production.

1.2.4 Market Segmentation by Grade

PMMA is supplied as either general purpose grade or optical grade. The grade of PMMA used in the automotive and construction industries is often general grade, while the specification of PMMA used in the electronics and signs and display industries is held to the standard of optical grade. The difference in the grade of PMMA lies in the composition of the monomers used in the polymerization process. Optical grade PMMA is produced by the free radical polymerization of solely MMA, resulting in a homopolymer, while general grade PMMA can be produced with polymerization of MMA along with other comonomer additives, producing a copolymer. Butyl acrylate is a commonly used comonomer added to increase the impact strength of PMMA[1]. Methacrylic acid is also a commonly used comonomer used to increase the glass transition temperature of PMMA[1].

1.3. PMMA Production Processes

1.3.1 Overview

PMMA is industrially produced in many countries across the world at a variety of plant capacities, generally ranging between 10,000 and 100,000 tonnes of PMMA per year. Plants in the USA, Taiwan, and elsewhere all currently use the same technologies for the production of PMMA by either incorporating the ACH process or Alpha process. Plants of similar technologies generally incorporate the use of the same unit operations at different specifications to produce the desired throughput of PMMA. In general, the specifications of these unit operations are often the same; for example, temperature and pressure conditions, unit operation types, and the general procedure for the production of PMMA is largely consistent between plants, making design of a plant easier.

PMMA is produced from the free radical polymerization of methyl methacrylate (MMA). The monomer, MMA, can be produced from a variety of processes. As seen in Figures 6 and 7 below, the Alpha Process is the most developed technology/route for producing MMA that has already been commercialized .

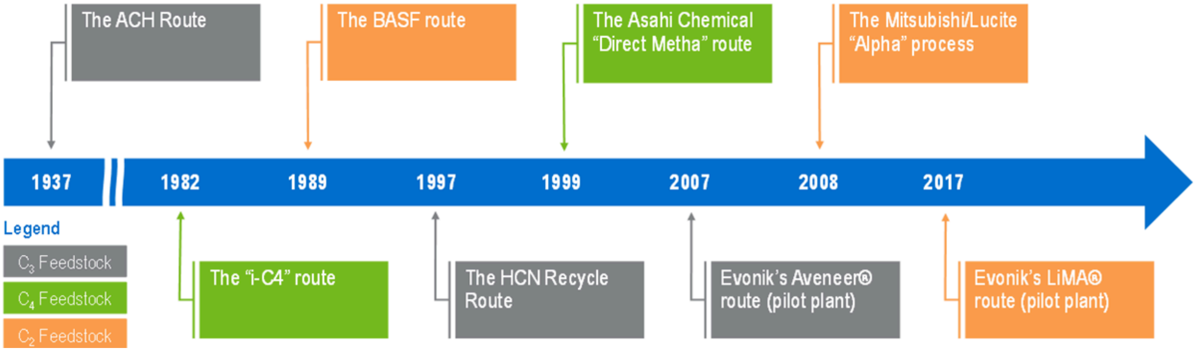


Figure 6: Various Routes for Producing MMA[21]

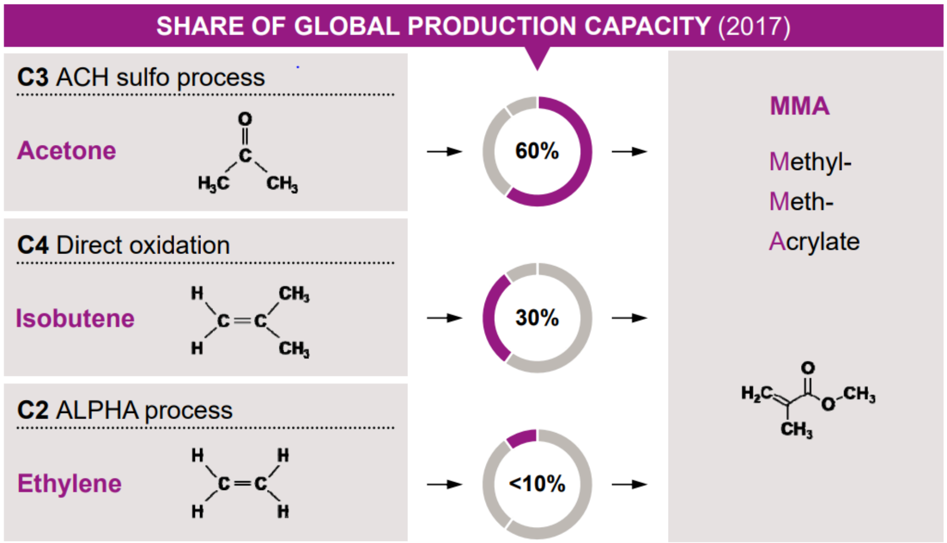


Figure 7: Production Capacity Segmented by Process Routes.[30]

1.3.2 Comparing Processes

Decision Matrix: Production Process

Considerations	Weighting	ACH	I-C-4	Alpha	LiMA
Feedstock Price	0.8	6	6	6	6
Waste Disposal	0.5	3	3	9	9
Feedstock Toxicity	0.4	3	6	6	9
EHS	0.9	3	6	9	9
Technological Feasibility	1.0	9	6	9	3
Efficiency	0.5	6	3	6	9
Total	-	22.2	21.6	31.8	28.5

Table 1: Production process decision matrix.

Scale of Scores:

3- Undesirable

6- Satisfactory

9- Optimal

In selecting the best manufacturing process of PMMA, several factors were considered and used to compare current and older processes (Table 1). One of the older processes and also the most popular, is the ACH process. OEAA opted not to undertake this path in the manufacturing process due to its toxic reactant HCN and a large amount of byproduct ammonium bisulphate (estimated at 1.2 kg for each kg of MMA), which is reprocessed to produce sulfuric acid. This step requires additional processing units and investments, which further decreases the favorability of the ACH process.

In considering the usage of the IC4 process, perhaps the most undesirable trait is the feedstock price. In comparison to the other methods, the price of isobutylene is considerably higher than ethylene. Additionally, this process is more environmentally friendly than that of ACH, but is overshadowed by the Alpha and LiMA processes. Also detrimental to the selection of IC4 is the analysis of its process efficiency; overall, the IC4 process is the least energy efficient of the three possible options[15].

As for the LiMA process, it has certainly proven to be a potential competitor to the Alpha Process. The LiMA process is primarily advantageous with regard to efficiency and feedstock price; however, the process is unproven as of yet and cannot be considered technologically feasible in its current state (still a pilot plant). The LiMA process and Alpha Process share many similarities with regard to feed stock prices and waste disposal.[20]

On the other hand, the Alpha Process presents a number of competitive advantages in the production of PMMA. First, the process has minimal societal and environmental risks compared to the ACH and IC4 processes. Furthermore, the Alpha Process has little byproduct output throughout the process, which minimizes waste disposal needs and presents a desirable advantage over the ACH and IC4 processes. One of the main distinguishing features of the two processes concerns the synthetic route for PMMA; although the feed materials are similar, the catalysts can play a huge role in the overall efficiency of the process. A green engineering principle that is often emphasized is maximizing efficiency; by analyzing candidate catalysts, and the supporting data on the process efficiency, the OEAA group can maximize the efficiency of the process[16]. By meeting this principle, byproduct formation can be minimized while selectivity and yield of PMMA can be maximized. Moreover, the primary advantage the Alpha Process possesses which makes it a more feasible option than the LiMA process, is its established and proven feasibility in industry with regards to scale-up opportunities and operational manageability.

1.3.3 Description of Alpha Process

The Alpha Process is an innovative way of producing MMA that has been prominently used in Asia in recent years. The key reactions can be split into two major steps[33] as shown below in Equations 1 and 2. The reaction starts off with ethylene, methanol, and carbon monoxide in the feed stream to produce methyl propionate as an intermediate. A metal catalyst is usually included to increase yield of MeP, and a separator is often implemented to recycle the catalyst with excess methanol back into the feed stream, while the product stream moves on to a fixed bed reactor or a fluidized bed reactor with formaldehyde to generate methyl methacrylate (MMA). MMA monomers are then further polymerized into PMMA through free radical polymerization. Other forms of PMMA with certain specifications can be made through cross polymerizing MMA with other monomers.

1. Carboxylation of ethylene to produce methyl propionate (MeP)

$$C_2H_4 + CO + CH_3OH \rightarrow CH_3CH_2CO_2CH_3 \qquad \text{(MeP)}$$ **Equation 1**

2. MeP is condensed with formaldehyde in a heterogeneous reaction step to form MMA

$$CH_3CH_2CO_2CH_3 + CH_2O \rightarrow CH_3(CH_2)CCO_2CH_3 + H_2O$$ **Equation 2**

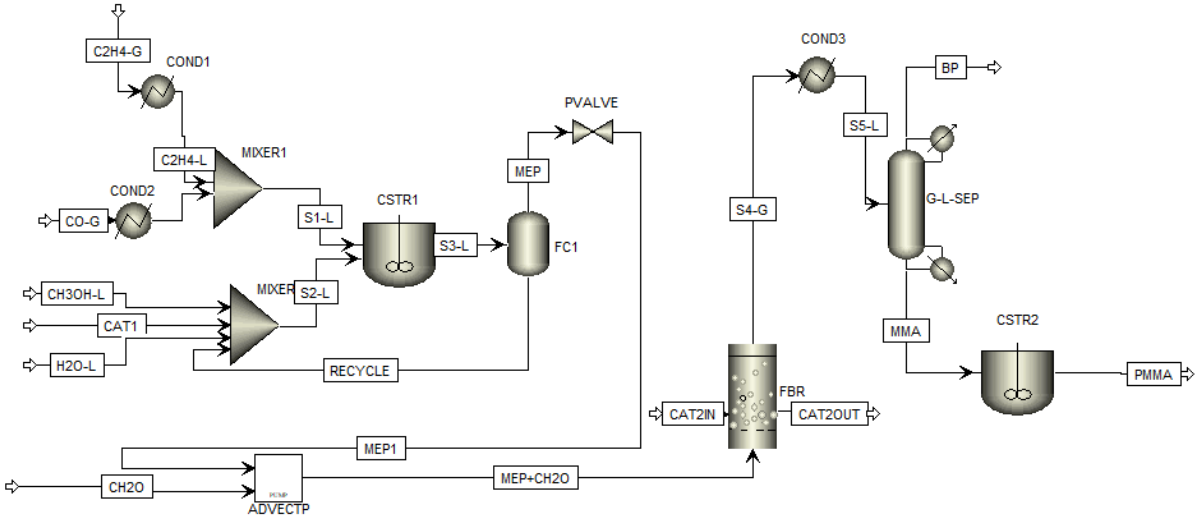


Figure 8: Preliminary flowsheet of the proposed Alpha Process[51-54]

Annotations:

-G: gas

-L: liquid

CAT: catalyst

COND: condenser

FC: Flash column

FBR: Fluidized Bed Reactor

G-L-SEP: Gas-Liquid Separator

ADVECTP: advection pump

BP: Byproduct

1.3.4 Value Chain

Extensive analysis of the general PMMA market, PMMA market segmentation by form, PMMA market segmentation by grade, and comparison of production processes for PMMA have been used to determine the encompassing value chain of the PMMA market.

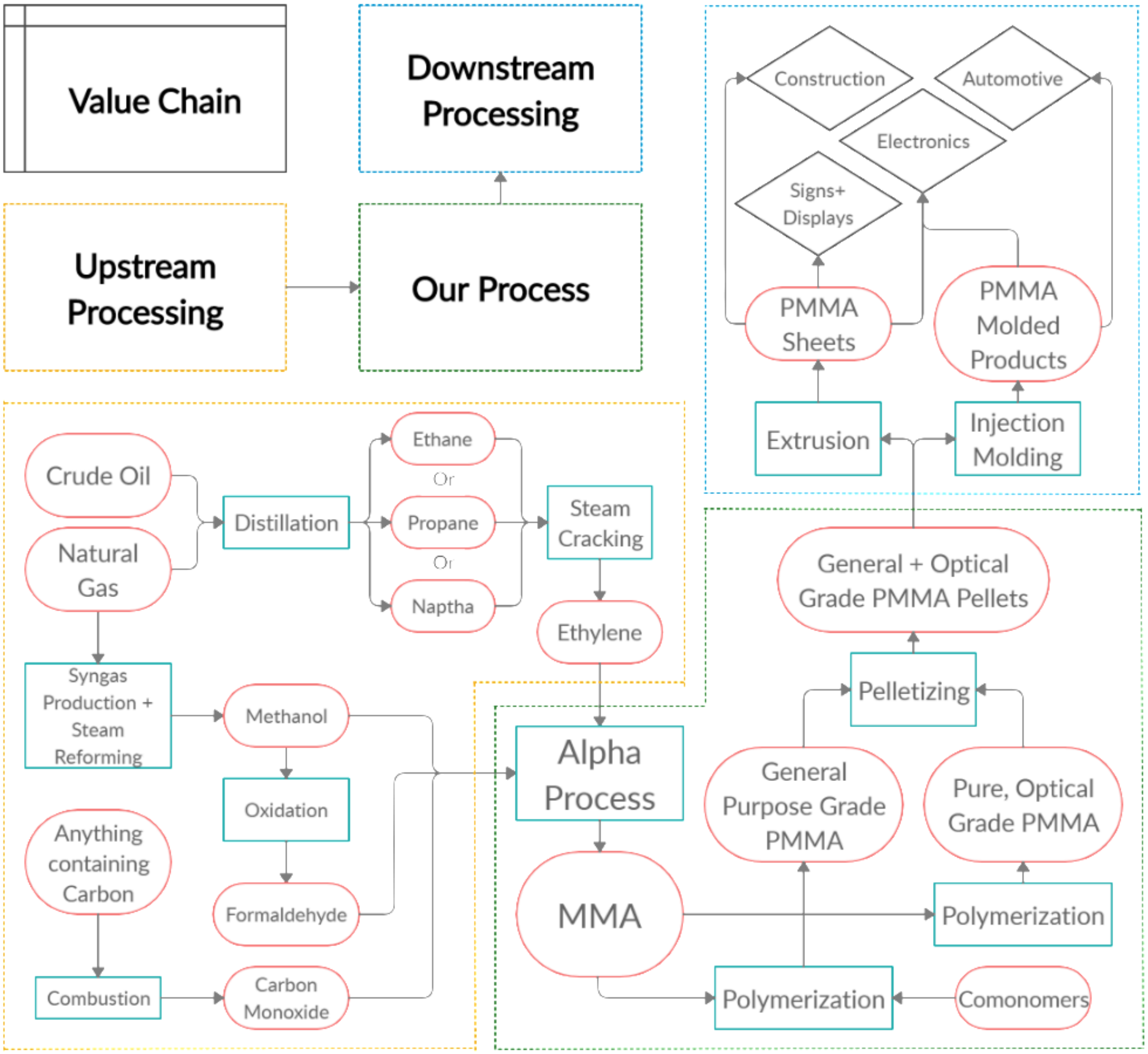


Figure 9: PMMA Value Chain.

1.4. Plant Location

1.4.1 Decision Matrix

Identification of an optimal plant location is contingent upon a number of factors, such as feedstock availability/pricing, regional market outlook, competition, and many more. It is essential that all the necessary considerations be made to suggest the most economically feasible plant location.

<u>*Country Abbreviations:*</u>

US - United States of America

SG - Singapore

JP - Japan

IN - India

CN - China

EU - Europe

SAU - Saudi Arabia

Considerations	**Weighting**	**U.S.**	**CN**	**SG**	**EU**	**JP**	**SAU**	**IN**
Feedstock accessibility/Price	0.8	3	6	6	3	3	9	3
Nearby Buyers	0.9	6	9	9	6	9	6	6
Regional Growth Rate	0.8	6	9	6	3	6	6	6
Land Price	0.5	3	9	6	3	3	9	6
Regulations	0.4	9	3	6	6	6	6	6
Taxes	0.3	6	6	3	3	3	6	6
Labor Price	0.7	3	9	6	3	3	6	9
Competition	1.0	9	6	3	6	6	3	6
Total	-	30.6	40.9	31.2	23.1	28.2	33.3	32.1

Table 2: Plant location decision matrix

Scale of Scores:

3- Undesirable

6- Satisfactory

9- Optimal

After thoroughly considering all the major factors identified in Table 2, the OEAA group has reached a consensus on locating its PMMA production plant in China. More specifically, the chosen location is in the Hefei economic and technological development zone located in Hefei, Anhui, the capital of Anhui province. The decision was made with the intention to maximize the SOM and minimize the overall capital and operating costs, while still maintaining the environmental and social sanctity in the area. One reason our plant location should be in China is primarily because China is the largest importer of PMMA, but also because local production in China is minimal with respect to the local demand for it. Additionally, a plant location in China is ideal due to nearby countries outside of China in the Asia-Pacific region that have a high demand for PMMA. According to a report from BCC research, the Asia-Pacific region comprises of 2.2 of the estimated 4.64 billion dollar global market, which equates to nearly half of the total global demand.[10] Feasibly, our Serviceable Addressable Market (SAM) in the Asia-Pacific could reach 2.2 billion dollars, with a large portion of this SAM likely coming from within China. Due to the large market volume of PMMA in the Asia Pacific region, and the secondary fact that China is the largest consumer and importer in the region of PMMA products, the decision to locate in China is justifiable. In addition, the case for setting the plant in China, is further strengthened by the recent implementation of new regulations favoring foreign investments, as the Chinese government looks to mitigate the detrimental effects that exist as a result of the on-going trade war[55].

1.4.2 Feedstock - Methanol and Ethylene

Coincidentally, China also happens to be one of the largest manufacturers of both ethylene and methanol, with methanol sold at a much lower price domestically compared to the remainder of Asia[29].

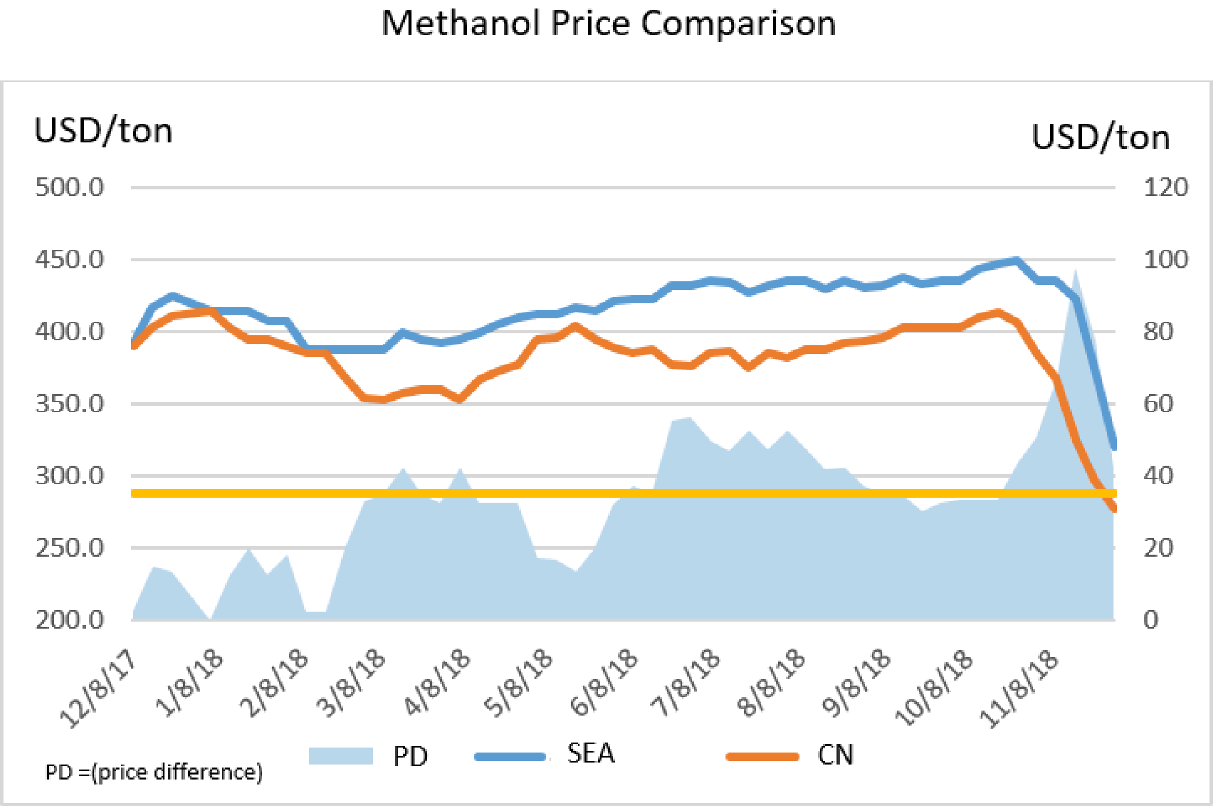


Figure 10: Comparison of price of methanol in China vs Southeast Asia[29]

An important consideration with respect to the location decision is feedstock pricing and accessibility, specifically with ethylene. As shown in Figure 9 in the Value Chain section, ethylene is derived from steam cracking of ethane, propane, and naptha, where all three precursors are from distillation refining of crude oil and/or natural gas. As discussed in Section 2.2, demand and import of PMMA in China has been higher than any other country. A similar statement can be made for ethylene, where imports to China have increased from 800 kilotons in 2010 to 2,600 kilotons in 2018; however, the recent startup of large-capacity ethylene plants across China indicates that reliance on ethylene imports could contract in 2020.[22] Historically, China has been utilizing their own naphtha steam crackers to produce ethylene themselves in order to rely less on imports; however, due to the shale gas boom and high production of cheap natural gas in the U.S., major petrochemical companies in China are starting to shift towards cracking U.S.-imported ethane in order to produce ethylene[23]. Although the recent trade war has increased the tariffs for ethane imports to China from 2% to 7%, many Chinese petrochemical companies are still starting up large ethane-cracking plants since they provide much larger margins than traditional naphtha crackers. One such company is Zhejiang Satellite, which has already started construction on a plant in Lianyungang in Jiangsu province that will produce 1.25 million tons of ethylene per year[24]. The Anhui province's presence next to the Jiangsu province provides a reason to expect a large, steady supply of ethylene at low transportation costs to a PMMA plant located in Hefei.

Overall, the Hefei economic and technological development zone was specifically chosen because of its high feedstock material accessibility, moderate competition, and relatively low capital and labor cost. The area of land benefits from being in the East China region, which has the highest ethylene production, representing 32% of the overall production in the country[41] (and is expected to grow with the startup of new ethane crackers in East China). It is also located in close proximity to Sinopec, the largest methanol manufacturer in China, which makes approximately 1.8 million tons per year[29]. While Hefei development zone as a whole is ranked 13th out of the 219 existing development zones in China based on output value in 2018[43], it has only started to direct its emphasis toward electronics, home appliances, and medical instruments by the end of 2013, and is currently still trying to recruit foreign investors.[45] With that said, producing PMMA at Hefei would be ideal, as it fits the profile toward which the development zone is pushing. Finally, with Hefei not located directly on the coast, and being a place that is not as developed as the first tier cities in China, the capital and labor cost are estimated to be on the lower end of the spectrum, which can help achieve our efforts in maximizing the profit.

With that said, even with the newly imposed regulations and tax relief policies toward foreign businesses, China has a track record of not fully honoring their agreement on the international stage.[56] Therefore, the nature of setting the operation units in China could still be relatively risky.

1.4.3 Serviceable Addressable Market (SAM) and Serviceable Obtainable Market (SOM)

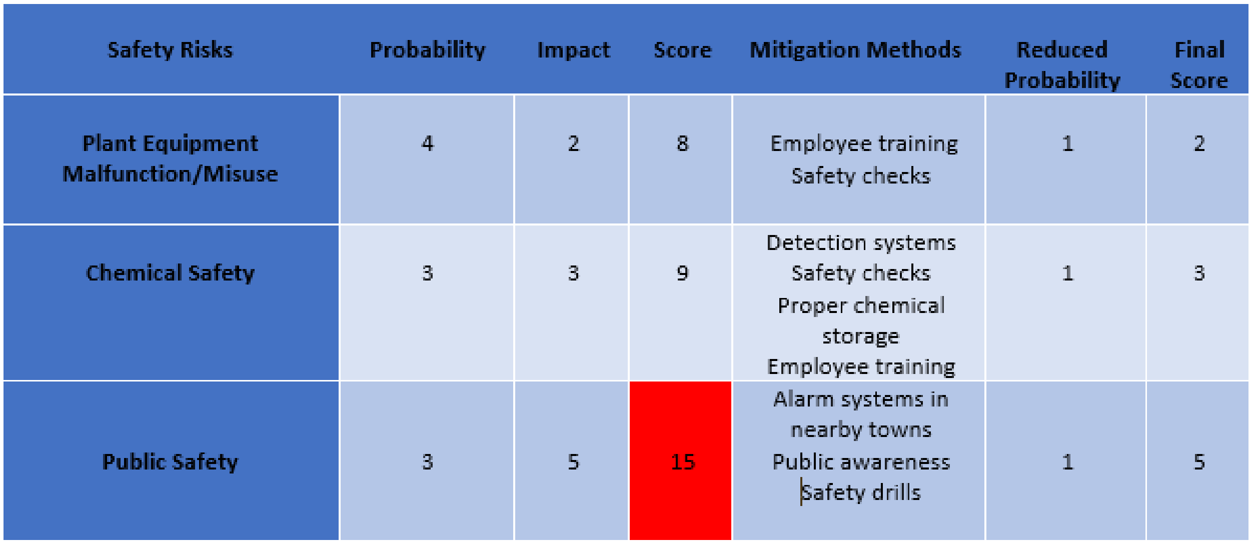
Now that the plant location has been determined and thoroughly justified, the SAM and SOM can also be formally addressed. First we look at a market-average derived SOM. Using the average capacity of 50,000 tonnes/year as an estimate for our plant capacity in conjunction with an average market price in Asia of $2500/tonne[36-40] for PMMA, the expected Serviceable Obtainable Market (SOM) is determined to be 125 million dollars.

Next, we verify our estimate above by comparing it with a top-down estimate of the SOM (what percentage of the SAM is our previously estimated SOM). As discussed in Section 2.2, the global market (or TAM) was found to be $4.8 B. According to Figure 3, China's own market encompasses 40% of the global PMMA market. Additionally, Figure 5 suggests that the pellet segment of the PMMA industry accounts for 73% of the PMMA market. Therefore, the PMMA pellet market in China (SAM) would be $1.4 B. Our previously estimated SOM of $125 MM would then only be 8.9% of this SAM value, which is plausible.

1.5. Risks

1.5.1 Safety Risks

The Alpha Process used for the production of PMMA has inherent safety risks associated with it, just as any chemical producing plant will. One obvious, but necessarily addressable risk is that associated with plant machinery. Plant machinery within the plant will operate at high enough temperatures to prevent safety threats to workers involved in the operation of this machinery. As such, it is necessary to take precautions as a means of mitigating risk through the installation of control systems which shutdown equipment exhibiting unsafe conditions such as unusually high temperatures, pressures, etc. Additional precautions may include frequent safety checks by government entities or supervisors, and the training and licensing of any individuals concerned with the operation of potential dangerous operating units. Additionally, chemical safety could prove a potentially dangerous risk if left unconsidered, especially with the use of carbon monoxide as an essential feed material. Carbon monoxide is undetectable by both color and smell and is deadly under prolonged exposure. Mitigation of the risks associated with using carbon monoxide can be accomplished by employing preventative measures such as the installation of carbon monoxide detection systems and ensuring that all employees are well-versed in handling all the chemicals involved in the production of PMMA. Aside from carbon monoxide, several of the chemicals used are flammable, so the storage of such materials needs to be done in such a way that minimizes the possibility of endangering employees. Furthermore, it is important to account for the safety of the public residing near the plant. Potential risks concerning the public include what would primarily be plant-wide failures, such as explosions or dangerous gas release. Assuming the necessary precautions are in place to protect the safety of plant employees, the probability of occurrence of either of these events is extremely low; however, it is necessary to install alarm systems throughout nearby cities in towns in the event that critically dangerous events occur.



Safety Risks	Probability	Impact	Score	Mitigation Methods	Reduced Probability	Final Score
Plant Equipment Malfunction/Misuse	4	2	8	Employee training Safety checks	1	2
Chemical Safety	3	3	9	Detection systems Safety checks Proper chemical storage Employee training	1	3
Public Safety	3	5	15	Alarm systems in nearby towns Public awareness Safety drills	1	5

Table 3: Safety risk assessment

1-5: Minimal Risk

6-14: Moderate Risk

15-25: Critical Risk

With regard to risk, the largest risk faced concerns the public safety of nearby towns and cities. Without the proper training by plant employees, in addition to a lack of public awareness, the probability of catastrophe is much more likely. Therefore, it is necessary that precautions are taken to prevent such a tragedy, especially because the impact of such an occurrence is very high.

1.5.2 Technical Risks

Particularly concerning the Alpha Process, there are several technical risks to be considered when weighing the viability of this option. Most importantly, it is necessary to enumerate the various processes used to produce PMMA aside from the Alpha Process. The most notable process currently in use in industry, the ACH process, uses acetone and hydrogen cyanide as feedstock. When contrasted with the Alpha Process, the ACH process lacks in a number of areas, especially with the amount of waste produced, as well as process efficiency. Technologically speaking, the ACH process poses little threat to the Alpha Process as a risk. However, another more recent innovation in the production of PMMA, which has been named the LiMA process, utilizes ethylene and methanol as feedstock, and overall is more energy efficient. However, its technology is relatively new, and it has not been tested in enough capacity to yet be considered a dangerous threat. Furthermore, the technology's current limitations prevent it from being a dominant method in PMMA production for the short term. In the event that the LiMA process were to overtake the market as the new dominant process for PMMA production, the risk can be mitigated by ensuring that the target market and plant location are carefully and selectively decided. Aside from the processes, it is necessary to consider the chemical natures of the constituent materials being used in the Alpha Process and how they may prove to be technical risks with respect to process control issues. For example, the MMA monomer has a strong propensity to polymerize, meaning that its polymerization occurs readily and easily in the proper conditions[33]. Considering that the anticipated goal of the PMMA plant is to produce a specific grade of PMMA, it is of paramount importance that the conditions of polymerization are well specified within the operation units handling the MMA. Similarly, the yield of the proposed process could vary depending on the synthesis route taken. In the production of PMMA via the Alpha Process, several routes exist by which the polymerization can occur, often contingent on the type of catalyst selected. The risk in making such a decision could be moderately large, but can easily be minimized by a simple analysis of a variety of catalysts usable in MMA polymerization. Finally, PMMA production could potentially be substituted by a better, more sustainable material that meets the same needs, but is more cost effective. The immediate impact of such a material would be small, but could weigh heavily on PMMA production decades down the line. The riskiest factor of such an event is the predictability of occurrence; substitute products in industry often enter markets unexpectedly, making the mitigation of such a risk difficult to handle. However, instead of addressing the issue of a new material, or improving our PMMA production as a whole, we can counteract the probability that a new material will impact the PMMA market by minimizing costs within the plant. This could be done by automating certain plant features, changing the feedstock supplier, producing the plants feedstock inhouse, etc. By doing so, it is possible to capture more of the value chain, making PMMA production more profitable, and less risky with respect to competing materials that meet the same standards as PMMA in the respective industries PMMA dominates.

Technical Risk Assessment

Technical Risks	***Probability***	***Impact***	***Score***	***Mitigation Methods***	***Reduced Probability***	***Final Score***
Competing Technologies	*4*	*4*	*16*	*- Optimal location selection* *- Target Market*	*2*	*8*
Process Control	*4*	*3*	*12*	*-Control Systems* *-Quality Control* *-Operation Unit Performance Tests*	*1*	*3*

Yield	*3*	*4*	*12*	*-Gather Data* *-Performance tests on unknown catalysts*	*1*	*4*
New Material	*2*	*4*	*8*	*-Minimize costs where possible* *-Insourcing instead of outsourcing*	*1*	*4*

Table 4: Technical risk assessment

1-5: Minimal Risk

6-14: Moderate Risk

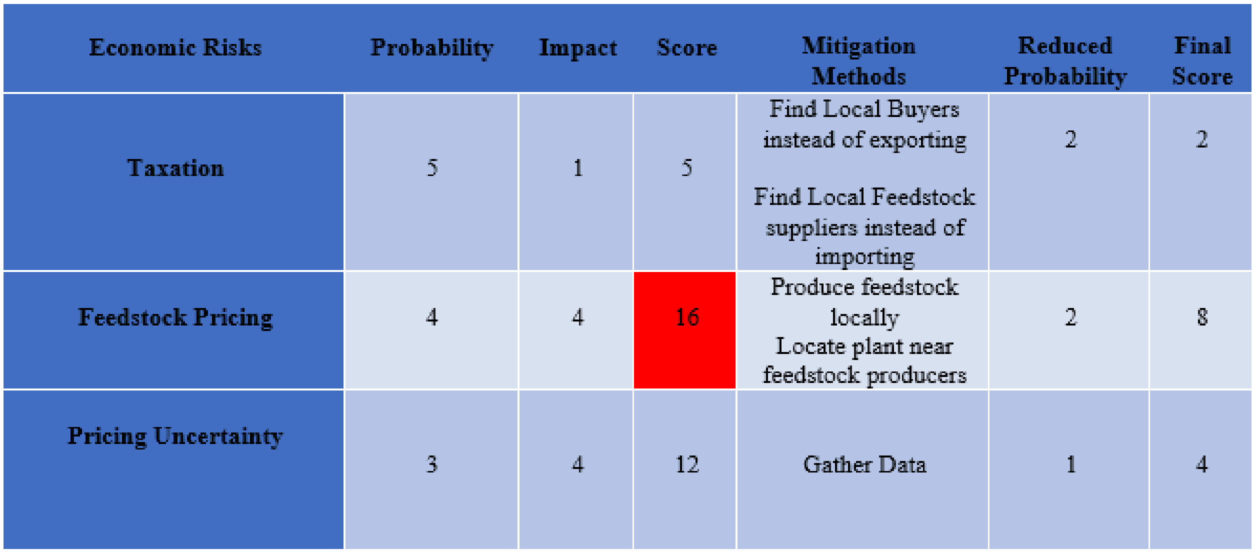
15-25: Critical Risk

Evidently, the most threatening technical risks are competing technologies and new materials in the market (Table 4). However, these risks can be dealt with by meticulously considering all the potential plant locations which would place OEAA in a position of competitive advantage, where new competitors would be unable to compete with the pricing offered by OEAA.

1.5.3 Economic Risks

As in any market, there are several economic risks to be considered before entering the PMMA market. Key economic aspects to consider in the production of PMMA pertain to taxation on exportation/importation, feedstock pricing fluctuations, selling price uncertainties, and feedstock sourcing uncertainties. The taxation resulting from imports and exports in China, exist just as they do in any other country, but to a different degree. Current economic conditions between China and other countries have resulted in a 5% increase in taxation on imported goods, suggesting that the feedstock prices would be more expensive when imported from foreign countries[50]. As such, the resulting impact of taxation on our product can be considered moderate, and can only be accounted for by purchasing feedstock locally. Considering the main sources of feedstock being Carbon Monoxide, Ethylene, and methanol, there is reasonable risk associated with the price fluctuations of our feedstock material, especially in the case of ethylene and methanol (see Section 4.2). Demand for natural gas and its products is on a steady rise, due to the increase in global demand for polymeric materials, which utilize simple hydrocarbons such as ethylene as a starting material for producing monomers[48]. The result of the increased demand correlates with an increase in price, which could be cause for concern in producing PMMA with ethylene as a feedstock. Fortunately, several options exist which can minimize the impact of the price fluctuations; plant location may be decided in such a way that the source of ethylene feedstock for the plant can primarily come from locally based ethylene producers. Furthermore, OEAA could potentially opt to introduce the production of key feedstock materials locally. Additionally, the selling price uncertainties certainly exist across the various countries which OEAA could predictably sell to. Although the number of competitors producing PMMA (especially in China) are minimal, there are still a variety of different plants producing the same product. However, the issue may easily be reconciled by identifying key PMMA producers in the region and analyzing the sales of PMMA by these producers as a guideline for potential pricing points for our product.

Economic Risk Assessment



Economic Risks	Probability	Impact	Score	Mitigation Methods	Reduced Probability	Final Score
Taxation	5	1	5	Find Local Buyers instead of exporting Find Local Feedstock suppliers instead of importing	2	2
Feedstock Pricing	4	4	16	Produce feedstock locally Locate plant near feedstock producers	2	8
Pricing Uncertainty	3	4	12	Gather Data	1	4

Table 5: Economic risk assessment

1-5: Minimal Risk

6-14: Moderate Risk

15-25: Critical Risk

The most risky economic consideration is the feedstock pricing (Table 5). With Ethylene being a necessary feed material in the production of PMMA, it is necessary that the region in which the plant is to be located has accessible feed materials. Else, the option to produce the feedstock locally also exists; however, this option is very constraining in where the plant may be located.

1.6. Quality Assurance

For all grades of PMMA pellets that are produced in our plant, Quality Assurance (QA) testing is critical. Based on three major producers of PMMA, OEAA team has identified 3 major specifications that must be assured: transmittance, impact strength, and heat-resistance [26-28]. All grades of PMMA pellets produced by the Alpha Process must have at least 90% total luminous transmittance, as measured with the standard ISO 13468-1 procedure; for optical grade PMMA pellets, light transmittance will be required to have at least 92% transmittance. All grades must also pass the Charpy impact strength test (notched) with at least 20 kJ/m^2, using the ISO 179/1eU standard. For high impact grade PMMA pellets with downstream use in construction and automotive industries, the impact strength will range from 25-120 kJ/m^2, depending on the requirements of the customer. Additionally, all grades must also pass the Thermoplastics Melt Mass-Flow Rate test using the ISO 1133 standard (with condition 13), where 3.8 kg of PMMA is melted at 230° C and the mass flow rate is measured. Since the glass transition temperature for PMMA is around 105° C, all grades must have a flow rate of less than 20g / 10 min. For heat resistant grade PMMA pellets with downstream use in the automotive industry, the mass flow rate will range from 0.5-5g / 10min, depending on the requirements of the customer.

Additional QA tests that are less critical to the performance of the PMMA pellets, but are still necessary, include the following but not limited to: tensile modulus, tensile strength, temperature of deflection under load, water absorption, refractive index, and Rockwell hardness[26]. By implementing quality assurance methods, OEAA hopes to meet green engineering principles by employing the principle of "Prevention instead of Treatment," which essentially promotes high yield processes, with little waste[16]. By ensuring that the product being produced meets all the standards necessary, OEAA guarantees the minimization of waste (in the form of wasted PMMA that does not meet grading requirements).

2. Design Phase

2.1 Introduction

Following up the market analysis of PMMA, it was necessary to begin the design of a plant geared toward producing MMA at a purity of 99.99% whilst also maximizing recovery. Following this, the ultimate goal is the production of PMMA at the desired grade-type. Aspen Plus V10 was used to simulate the overall plant design, and to determine feasibility of such a design.

2.2 Methodology

2.2.1 Overview of Methodology

A number of key operations were necessary to be considered in the design of the plant. The types of unit operations utilized in the plant were each determined based on a number of key considerations; primarily, it was important that the simulation software accurately models unit operations in the intended way (i.e. simulation is representative of reality and is free of errors). Additionally, it was necessary to implement the most efficient operations into the design of the plant, primarily because these are the operations that will produce the most profit, but also because such operations are likely to minimize waste and maximize the recovery of our target products. As such, target goals within plant design were accomplished by analyzing the methodology applied in industry from similar PMMA producing plants. In the design of the plant using the Alpha Process, the most important considerations, and those to be discussed, concern the production of methyl propionate, the production of MMA, the separation of MMA and H_2O to achieve the target purity in the monomer, the polymerization of MMA to produce the final target product of PMMA, and finally, the extrusion of PMMA into the desired product of PMMA pellets.

2.2.1 Production of Methyl Propionate

The production of methyl propionate with carbon monoxide, ethylene, and methanol is a commonly-researched reaction in industry.

Figure 11: Reaction stoichiometry to produce Methyl Propionate

As such, finding accurate and specific reaction kinetics for this particular step was simple. An analysis of the reaction rate equation revealed that the method that is most optimal for maximizing the conversion of methyl propionate involves maximizing the concentration of methanol.

$$R = \frac{K_1 \cdot K_2 \cdot k_3 \cdot [Pd] \cdot [CO] \cdot [C_2H_4] \cdot [MeOH]}{1 + K_1 \cdot [C_2H_4] + K_1 \cdot K_2 \cdot [CO] \cdot [C_2H_4]}$$

Parameter	**Final Value**
k_3 [mL/mol/min]	7.913E01
K_1 [mL/mol]	9.791E04
K_2 [mL/mol]	1.071E9

Figure 12: Reaction rate law for the production of methyl propionate and relevant parameters

A CSTR was chosen in this portion of the design due to its ease of operation as well as it being the most commonly used reactor in industry for this particular process. After simulation, the conversion of the limiting reagent, ethylene, was found to be 99.99%, producing the desired amount of methyl propionate for the following step.

2.2.2 Production of MMA

The next step after producing MP is the gaseous catalytic reaction of methyl propionate MP with formaldehyde to produce MMA and H2O. The most commonly used reactor type in industry for this particular process is a packed bed reactor; however, recent research has shown that a fluidized bed reactor, where the solid bed is suspended/fluidized rather than stationary, can yield higher conversion of MP and formaldehyde. Reaction kinetics for this particular process were not found; instead a kinetics law was derived by using data from an academic paper [75] (which detailed conversions of MP in a lab-scale FBR at different temperatures), and then replicating the lab-scale FBR in Aspen to find the reaction constant k that gives a specific conversion at a specific temperature (assuming an elementary rate law of the form r =

k*[MP][Forma]). Lastly, a linearized Arrhenius plot was created to obtain the kinetics parameters k0 and Ea. See Figure 13 below for the linearized Arrhenius plot, which shows a relatively strong linear trend.

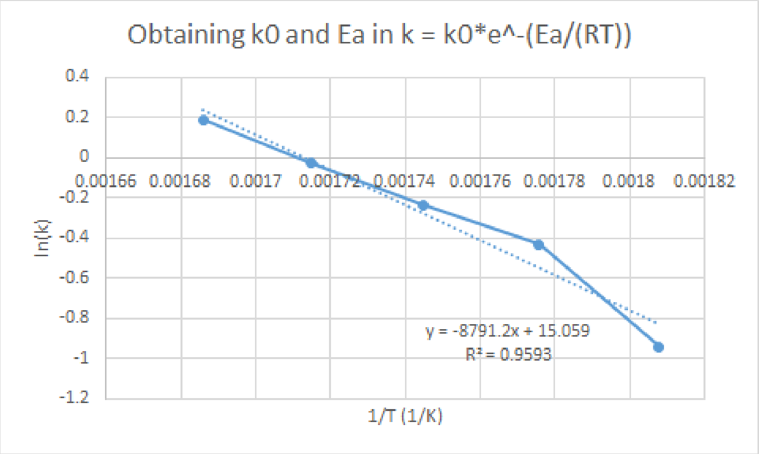


Figure 13: Linearized Arrhenius Plot

For the design of the FBR, three critical assumptions that were made are: 1) the conversion can increase over the limit described in the paper as long as the fluidization regime, molar fractions of reactants, and solids volume fraction remains constant during scale-up, 2) the solids volume fraction required in the FBR is inversely proportional to the residence time, and 3) the reaction pressure can be slightly higher than 1.013 bar. Assumption 1 is justified since with any kind of reactor, increasing the volume will almost always increase the conversion of a reaction due to a higher residence time (and the selectivity should remain the same if the temperature is the same). Assumption 2 is justified since a longer residence time could potentially relate to a lower requirement on the amount of solids catalyst needed in the FBR. Assumption 3 is justified since the paper cited never mentioned a reaction pressure; however, even though the lab FBR from the paper was most likely performed at 1 atm, it is known that aldol condensation reactions in general can range from 1 bar to 3 bar in industrial FBRs [76]. Unlike the first reaction that produces MP, the reaction in the FBR is only 86.1% selective to MMA and produces byproducts. Since reaction kinetics for byproducts formation are unavailable in any public literature, two RStoic units were used to convert the necessary fraction of MP to byproducts (two units were required to allow the stoichiometry to be a function of inlet stream composition).

2.2.3 Separation of MMA to Target Purity

The most difficult obstacle in the design of a plant using the Alpha Process was the separation of MMA and H_2O. The preliminary design flowchart in Figure 8 assumed a simple separation achievable by a rudimentary distillation process; however, it was found that the mixture leaving the FBR had a fairly equal composition of water, methanol, and MMA, where MMA and H_2O with a 0.1°C difference boiling point at 1 atm. As such, a more complex approach was taken in the separation of the two. Specifically, a liquid liquid extraction was performed using an extractor accompanied by pentane as a solvent. In short, the pentane was used to create two immiscible liquid phases: one aqueous phase containing water, and the other phase containing organic pentane and MMA. Following this, MMA was purified in a number of distillation steps removing key components in the mixture resulting from the FBR, while also incorporating the separation of pure pentane for recycling as well as the purification of methyl propionate at a target purity of 98% to be sold as a byproduct of the plant. Ultimately, the three distillation steps accomplished the separation of MMA from all other components at a purity of 99.99% as well as a recovery of 94.62% from the FBR outlet stream.

2.2.4 Polymerization of MMA

The final step in the polymerization of MMA to produce PMMA required a CSTR accompanied by a solvent and initiator to perform solution polymerization. Specifically, ethyl acetate and azobisisobutyronitrile were selected as our solvent and initiator, respectively. These particular chemicals were chosen primarily because the simulation program, Aspen Plus, already contained the complex reaction kinetics associated with this polymerization reaction (Appendix A).

2.2.5 Extrusion of PMMA Pellets

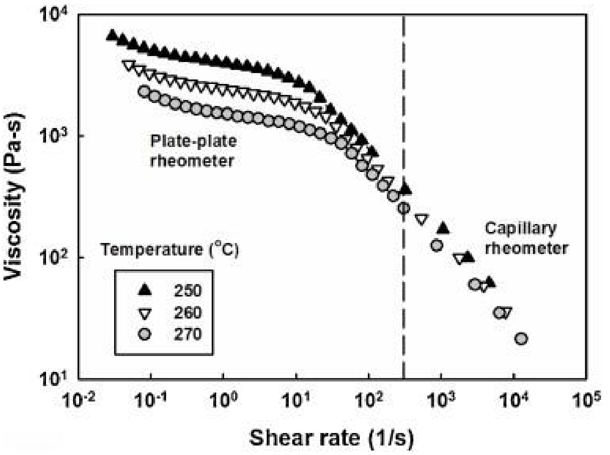


Figure 14: Relationship between Viscosity and Shear rate for PMMA derived from experiment.[58]

Team OEAA a single screw extruder over a twin screw extruder for the extrusion of PMMA due to the low temperature sensitivity of PMMA. The extrusion of PMMA usually operates at the temperature range of 210◦ C to 260, ensuring that the material is extruded far enough from the glass transition temperature (at 100◦ C). The extruders designed for our plant are set to operate at 250◦ C. Multiple extruders were designed to accommodate for PMMA flowing in at different viscosities, and the corresponding shear rates were determined accordingly based on Figure 14. Due to the difficulties in getting a literature value for K, the die constant, we have attempted to use the mass flow rate of each extruder with an estimated pressure drop across the extruder to back calculate K. The extruder length and diameter (L/D) ratio is set to be 36:1, with the diameter being 90 mm. The helix angle was set to be 17.656◦, which would make it a square pitch screw. The height and width of the screw channel was specified as 1 mm and 5 mm respectively, which gave F_d and F_p values of 0.90 and 0.88 respectively according to Figure X. Finally, all of the calculated and specified parameters were linked together using the screw characteristic equation shown in Equation X.

$$\dot{m} = \rho Q = \frac{WHv_b \cos\theta}{2} F_d - \frac{WH^3}{12\mu}\left(\frac{\Delta P}{Z}\right) F_p$$

Figure 15: Used to determined the specifications for the designed extruder

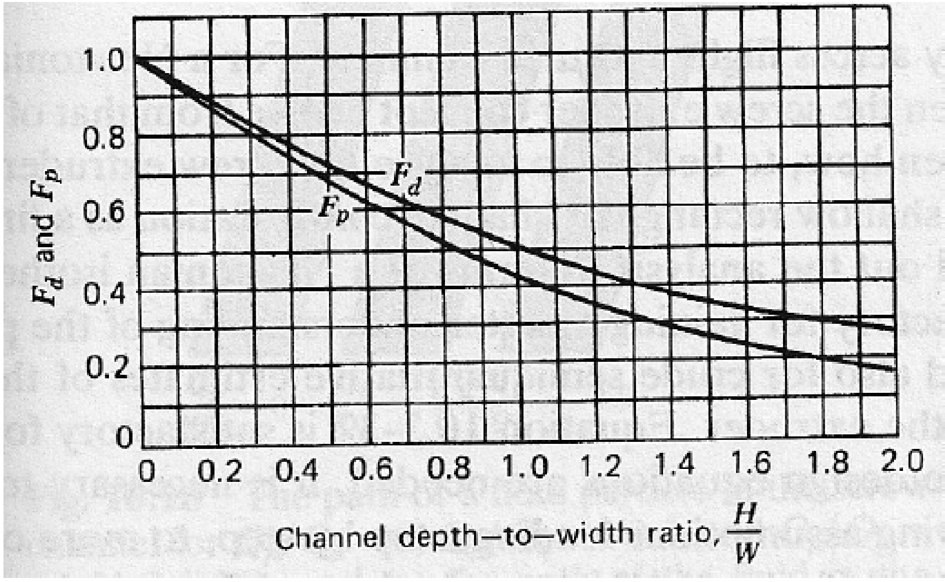


Figure 16: Shape factors for screw channel flow

2.3 Results

2.3.1 Flowchart and Design Basis

The flowchart for the plant is included in Figures A4a and A4b in the appendix. The equipment specification sheets are included in Figures A5 through A19 in the appendix. The design basis sheet and stream tables are included in the submitted final deliverable.

2.3.2 Utilities

Table 6 below shows the overall utility requirements per year.

Utility Type	Rate	Units
Electricity	2154	kWh/yr
HP Steam	4.7E+05	MMBtu/yr
MP Steam	2.8E+06	MMBtu/yr
NG Heating	7.5E+04	MMBtu/yr
Cooling Water	2339	MMGal/yr
Refrigeration	854	klb/hr

Table 6: Utilities Information

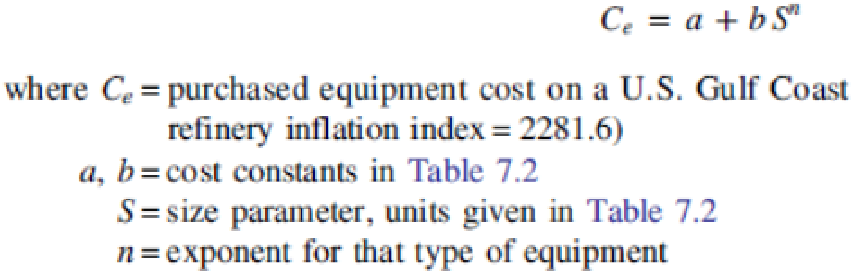
All rates are calculated assuming a 90% efficiency in the delivery of the utilities. Electricity includes the work required by the compressors, pumps, and extruders. HP (high pressure) steam is at 444.6 °F and 400 PSI and is used for some of the heaters and reboilers of the distillation towers. MP (medium pressure) steam is at 327.8 °F and 100 PSI and is used for some of the heaters and reboilers. HEATER4, which is used to heat the stream before entering CSTR2 (the polymerization unit) to 500 °C, requires a furnace that relies on natural gas as fuel. Cooling water is used in the chillers and condensers of the distillation towers. For colder streams that need cooling, Freon-12 is used as a refrigerant. See Table A1 in Appendix A for detailed information on how the utilities are distributed to each unit operation.

3. Economics

3.1 Capital Expenses

3.1.1 Equipment Cost and Installed Equipment Cost

Two primary methods were used to obtain the cost of equipment (C_e) for each unit operation in the plant. Method 1 involves using equipment cost correlations from Towler (2013) [77].



$$C_e = a + bS^n$$

where C_e = purchased equipment cost on a U.S. Gulf Coast refinery inflation index = 2281.6)
a, b = cost constants in Table 7.2
S = size parameter, units given in Table 7.2
n = exponent for that type of equipment

Figure 17: Equipment cost correlations from Towler

For equipment not listed in Towler, cost correlations were found through online resources. As a last resort, Method 2 involves using cost estimations from Aspen Process Economic Analyzer (APEA). Since the process used in the plant is a re-design of an already existing process, a design margin of 1.07 was used for all process equipment size (i.e. S in the correlation is multiplied by 1.07 before being used in any correlation). For any equipment outside a valid range for S, the following equation was used:

$$\frac{\text{Cost A}}{\text{Cost B}} = \left(\frac{\text{Size A}}{\text{Size B}}\right)^n$$

Figure 18: Equation for equipments costs/sizing with values out of range for S

The exponent n was assumed to be 0.6 when it was not available (which is generally valid for all types of equipment). The installed cost (C_i) is simply the equipment cost multiplied by the install factor. The install factor for each equipment was determined using the factors detailed in Figure 19. Table 7 below shows the equipment cost C_e as well as the installed cost C_i for each equipment.

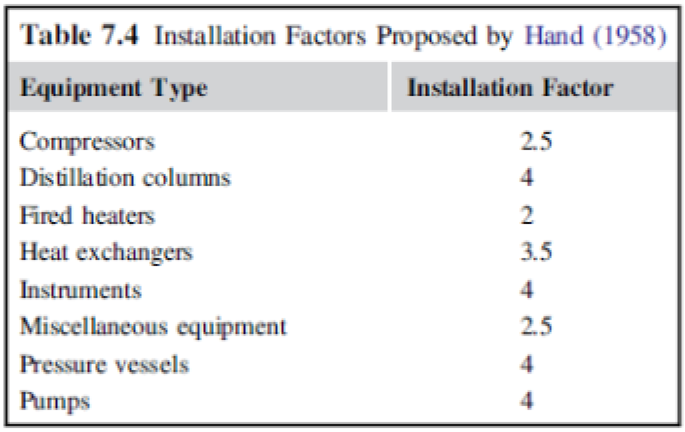


Table 7.4 Installation Factors Proposed by Hand (1958)

Equipment Type	Installation Factor
Compressors	2.5
Distillation columns	4
Fired heaters	2
Heat exchangers	3.5
Instruments	4
Miscellaneous equipment	2.5
Pressure vessels	4
Pumps	4

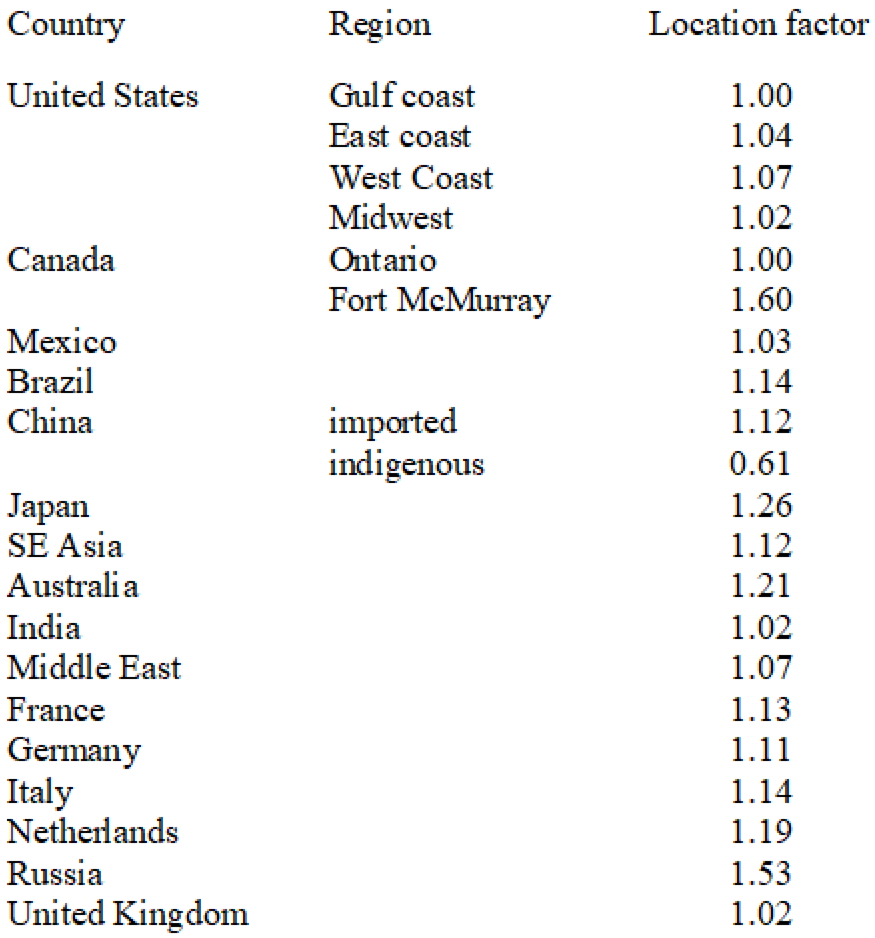
Figure 19: Towler Table 7.4 on Installation Factors for Variety of Different Equipment

Unit Op Name in Aspen	**Method**	C_e **(\$ MM)**	**Install Factor**	C_i **(\$ MM)**
FBR	[78],[79],[80]	48	3	143
CSTR1	1+2	4	3	11
MCOMPRES	1	3	2.5	7
EXPANDER	1	2	2.5	4
COMPRESS	1	2	2.5	4
CSTR2	1+2	1	3	4

Table 7: Capital Expense (purchased and installed) of Most Costly Equipment

The costs of all equipment using the methodology described are found in Table B1 (Appendix). Note that SPLITR1 and SPLITR2 are not part of the actual process (so they aren't included in the CapEx), since they are just there to facilitate convergence by limiting the amount that is recycled before the final run.

The total Inside Battery Limits (ISBL) is the sum of C_i and is equal to $189 MM; however, a time and location factor must be used to obtain the actual ISBL. The equipment cost was assumed to be from U.S. sources. The factors found in Figure 20 were used to obtain the location factor for buying equipment from indigenous China.



Country	Region	Location factor
United States	Gulf coast	1.00
	East coast	1.04
	West Coast	1.07
	Midwest	1.02
Canada	Ontario	1.00
	Fort McMurray	1.60
Mexico		1.03
Brazil		1.14
China	imported	1.12
	indigenous	0.61
Japan		1.26
SE Asia		1.12
Australia		1.21
India		1.02
Middle East		1.07
France		1.13
Germany		1.11
Italy		1.14
Netherlands		1.19
Russia		1.53
United Kingdom		1.02

Figure 20: Location Factors

The time correction factor is used to account for different prices of equipment at different time periods. Usually, a reference cost and reference index value is obtained from CE (Chemical Engineering) Journal for each type of equipment; however, since the cost of all the equipment comes from many varying sources (most without a year or index value), an overall time factor of 1.1 was assumed. So, the total correction factor would be 0.62*1.1 = 0.682.

After correction for location and time, the total ISBL cost is $129 MM.

OSBL costs were determined on the basis that our desired plant construction would be built on a new site for the production of a typical large volume chemical. The OSBL cost was estimated to be 40% of the ISBL, as suggested by Towler's table 7.8, and amounts to $36.3 MM.

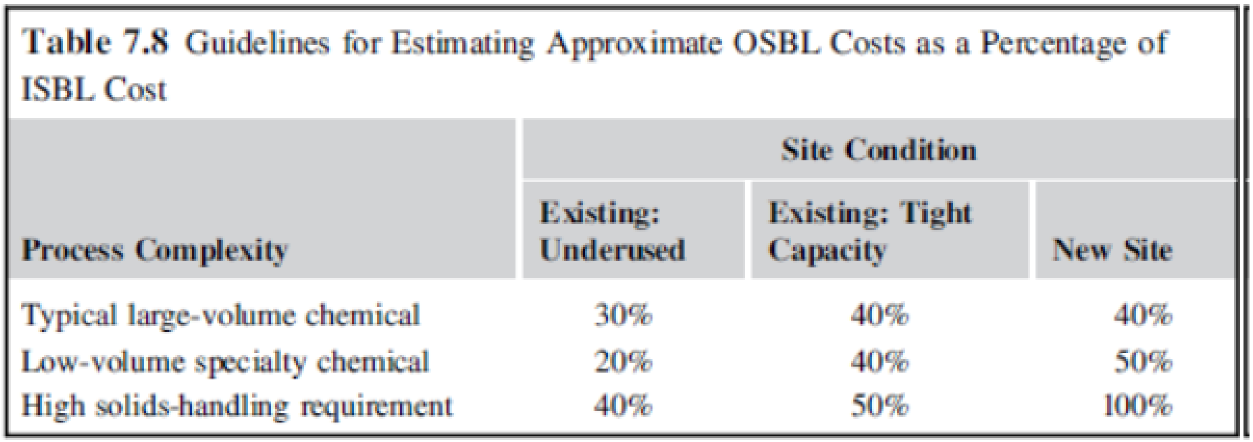


Table 7.8 Guidelines for Estimating Approximate OSBL Costs as a Percentage of ISBL Cost

	Site Condition		
Process Complexity	**Existing: Underused**	**Existing: Tight Capacity**	**New Site**
Typical large-volume chemical	30%	40%	40%
Low-volume specialty chemical	20%	40%	50%
High solids-handling requirement	40%	50%	100%

Figure 21: Table 7.8 from Towler

For the determination of engineering costs, most of the calculations were based on the industrial familiarness with the desired Alpha process. The alpha process has been commercialized for several years and is a well known process, but not necessarily an easy one. Due to the complicated nature of the Alpha process, the engineering costs were estimated to be between 20% (for known process) and 30% (for new process) = 25% of the ISBL + OSBL. These costs are estimated to cover design, procurement, construction oversight, and project management.

The total Engineering cost is: $36 MM

Similar to Engineering costs, the contingency costs were calculated based on a correlation of the ISBL and OSBL values. The contingency cost was determined to be 35% of the ISBL+OSBL cost. The uncertainty of the technology in the process required that a high amount of funds be placed aside in case of changes in scheduling and production.

The total Contingency cost is: $76 MM
The total fixed capital cost for just equipment is $295.3 MM

3.1.2 Additional Capital Expense

Inventory capital expenses include the use of recyclable solvent as well as catalysts that can be regenerated. Due to the nature of these products, they only require a one-time purchase in the desired amount necessary. These include the catalysts used in the CSTR1 producing Methyl Propionate as well as the catalyst used in the FBR producing MMA. The solvent needed for the LLE (liquid-liquid extraction) separation of MMA is pentane and is necessary in the process. The prices for each of these materials were found using several sources (listed in [83]) and the total cost was determined by multiplying the unit price of materials to the total amount needed for the plant throughput. 99% of the total inventory capital cost is from catalyst prices (split fairly evenly between the two types of catalysts) and the other 1% is the pentane solvent.

The total Inventory Capital Cost is: $3 MM

Based on data from several existing plants with similar output production, we estimate our physical plant and equipment to take up approximately 4000 m^2 of land, and we plan to purchase a total of 40000 m^2 of land for each operating unit to be properly spreaded out.

The land price listed at Hefei technological and economic development zone is at 3500 chinese yuan per m^2, which is equivalent to 494 USD/m^2. So the total cost of 40000 m^2 of land would turn out to be 19.76 MM. In addition, the property tax (which comes at 63.62 per m^2) will add an additional 2.54 MM.

The total land cost is: $22.3 MM

The total Miscellaneous Capital Cost is: $25.3 MM

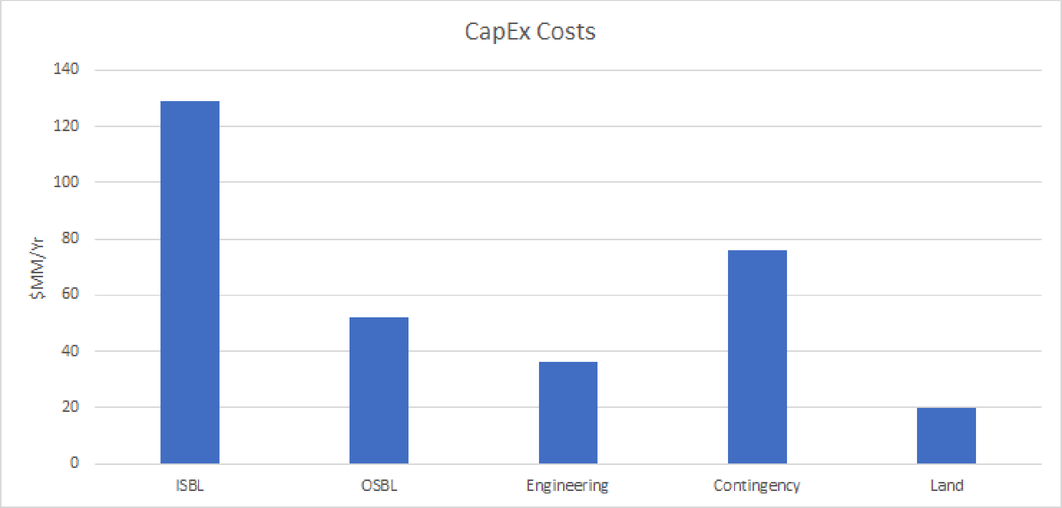


Figure 22: Capital expense costs

The total fixed capital cost is $318.5 MM

3.2 Operating Expenses:

3.2.1 Raw Materials:

Prices for raw materials were found through various sources (located in the list of sources under [83]) and are shown in Table 8 below. Most sources were market reports/articles, some were from vendors (prices were divided by a margin of 20-30% to account for buying in bulk), and one source was from a bottoms-up analysis (production cost of CO multiplied by a 20% markup margin).

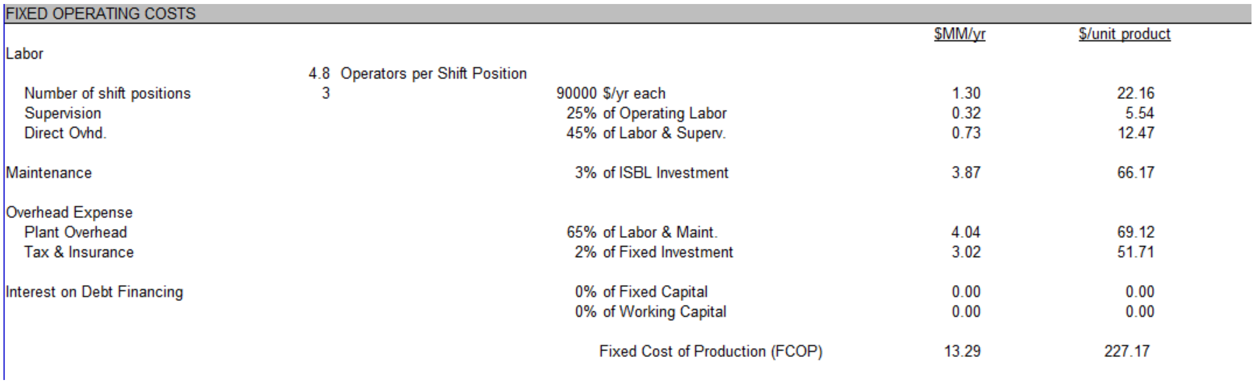
Raw Materials	Price ($/metric ton)	$MM/yr
Ethylene	513	13
Methanol	296	26
CO	268	7
ParaFormaldehyde	553	15
Pentane	1361	23
EA	937	0.8
AIBN	5292	2

Table 8: Cost of raw materials for the entire plant

An important assumption made was that Ethylene can be bought domestically in China from nearby ethane-cracking plants (so no import or overseas freighting fees). Another assumption was that all feedstock efficiency is 0.95 (i.e. 5% is lost on transport to the plant). The last assumption was that paraformaldehyde will be purchased since it can fully dissociate into formaldehyde in the methanol-rich inlet stream [75] and because it would be unwise to introduce an aqueous solution of formaldehyde (such as formalin) into the FBR (Le Chatlier's). Note that the pentane price is based on the amount that is not recycled (26 kmol/hr not recycled out of 350 kmol/hr total running through the plant). Also, in the cost_of_production, EA, AIBN, and pentane are considered consumables since they aren't direct feedstocks.

The total estimated Raw Materials+Consumables cost is: $87.9 MM/Yr

Fixed Operating Costs:



FIXED OPERATING COSTS					
				$MM/yr	$/unit product
Labor					
	4.8		Operators per Shift Position		
Number of shift positions	3	90000	$/yr each	1.30	22.16
Supervision		25%	of Operating Labor	0.32	5.54
Direct Ovhd.		45%	of Labor & Superv.	0.73	12.47
Maintenance		3%	of ISBL Investment	3.87	66.17
Overhead Expense					
Plant Overhead		65%	of Labor & Maint.	4.04	69.12
Tax & Insurance		2%	of Fixed Investment	3.02	51.71
Interest on Debt Financing		0%	of Fixed Capital	0.00	0.00
		0%	of Working Capital	0.00	0.00
			Fixed Cost of Production (FCOP)	13.29	227.17

Table 9: Detailed fixed operating costs

Fixed operating costs include the salaries of employees as well as direct overhead, insurance, and maintenance costs. The constructed plant is expected to require a total of 3 operators and 4.8 shifts per position. The number of supervisors needed is 1 per shift position. In order to incorporate direct overhead, the salaries of operators are assumed to be 90,000 $/Yr, with the supervisor positions totalling to 25% of the total yearly cost of all operator positions. The direct overhead is assumed to be approximately 45% of the total labor costs. In addition to this, plant overhead, maintenance, and insurance costs are found using correlations as percentages of ISBL and/or OSBL. Maintenance yearly costs are determined to be 3% of the initial ISBL investment, plant overhead is determined to be 65% of the labor and maintenance costs, and insurance is determined to be 2% of the ISBL and OSBL costs.

The total estimated Fixed Cost is: $13.29 MM/Yr

3.2.2 Utilities and Waste

Table 10 shows the price of utilities based on the type of utility. All unit operations are assumed to have a 0.9 efficiency in terms of how many units/hr of utility are needed.

Utility	Units	Units/hr	$/Unit	$MM/yr
Electric	kWh	2154	0.08	1.489
HP Steam	kg	8191	0.0137	0.97
MP Steam	kg	48562	0.0168	7.049
NG for Furnace	MMBtu	8.71	1.96	0.15
Cooling Water	MMGal	0.271	2500	5.854

Table 10: Pricing for Utilities Cost

For electricity, the rate is simply the power that's needed. The Units/hr Pricing for electricity was determined based on the pricing of electricity in the Hefei Province, China. For steam, HP (high pressure) steam is at 444.6 F and 400 PSIa while MP (medium pressure) steam is at 327.8 F and 100 PSIa. The enthalpy change from water at 25c and 1 atm to the needed conditions was multiplied with the mass flow rate needed through each unit operation; then, it was assumed that natural gas at a price of $1.96/MMBtu was used to supply the heat (the capex of the boiler and steam distribution system are assumed to be covered by the OSBL). For Heater 4, since the stream needs to be heated to 500c, steam cannot be used and so a furnace is used (capex is included in total cost) with an assumption of $1.96/MMBtu for heating the furnace with Natural Gas. Cooling water rate is simply the flow rate from Aspen and the pricing is based on the listed price of $0.0025/gal.

The total Utilities yearly Cost is: $15.3 MM/Yr

Waste:

The proposed plant design produces waste primarily composed of chemicals such as formaldehyde, methanol, carbon monoxide, and ethylene (which cannot be feasibly separated and recycled). The resulting waste is assumed to be disposable at a rate of 50 $/tonne.

The total waste disposal yearly cost is: $4.80 MM/Yr

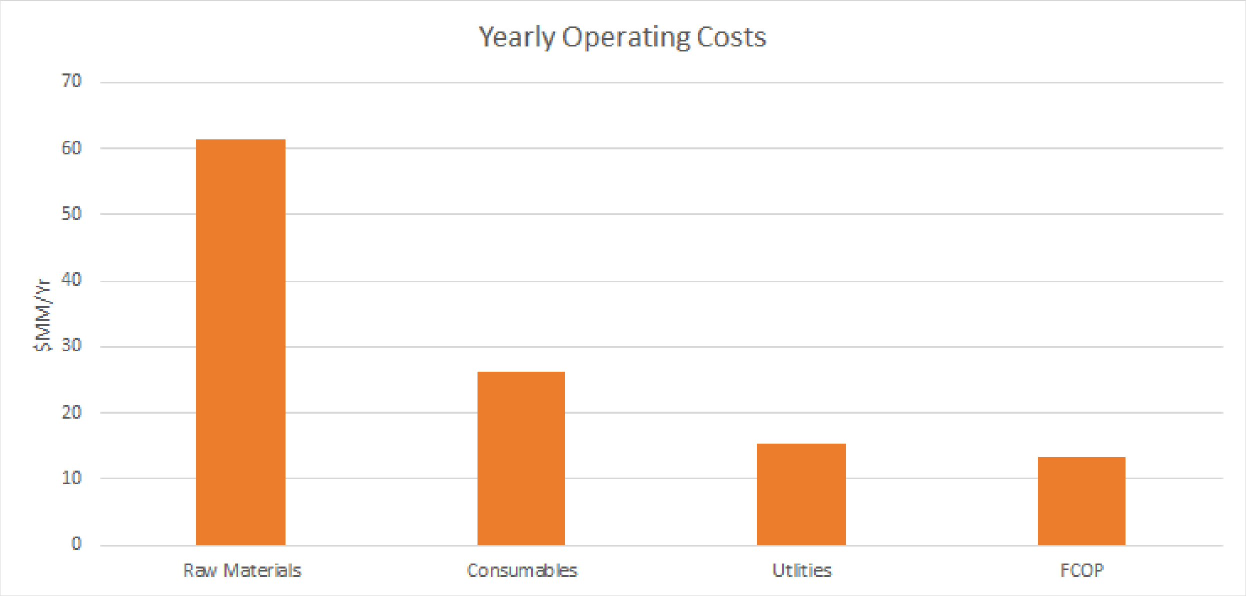


Figure 23: Yearly operating costs for different components

The largest factor impacting the yearly operating cost of the proposed plant design is primarily sourced from the feedstock used.

The total yearly operating cost is: $116.5 MM/Yr

The total operating costs (variable costs of production) are: $72.62 MM/Yr

3.3 Cash Flow Analysis

3.3.1 Depreciation and Taxes:

Depreciation of the plant was calculated using the total leverage, equity, cost of debt, and cost of equity.

Cost of Equity	10%
Cost of Debt	5%
Equity	30%
Leverage	70%

Table 11: The resulting weighted average cost of capital (WACC), was determined based on the following equation

$$WACC = x_{debt} \times Cost\ of\ Debt + x_{Equity} \times Cost\ of\ Equity$$

Thus, our weighted average cost of capital was determined to be 6.5%, indicating that the depreciation in the value of our plant and production would be a compounded 6.5% yearly rate.

Taxation in China follows a standard 25% yearly rate. However, the decision to locate the plant in the Hefei economic and technological development zone was partially considered due to the tax deductions presented by the Chinese government to foreign businesses in the area. Namely, China taxes new companies in the area at a rate of 15% for the first ten years of production. After the break-even point is reached, no tax is collected for the following two years. The following three years are then taxed at a rate of 12.5%, and the remaining years thereafter are returned to the usual 15% tax-rate. The cumulative tax incurred by the end of the project lifetime is determined using these taxation rates.

The total tax incurred: $156.1 MM

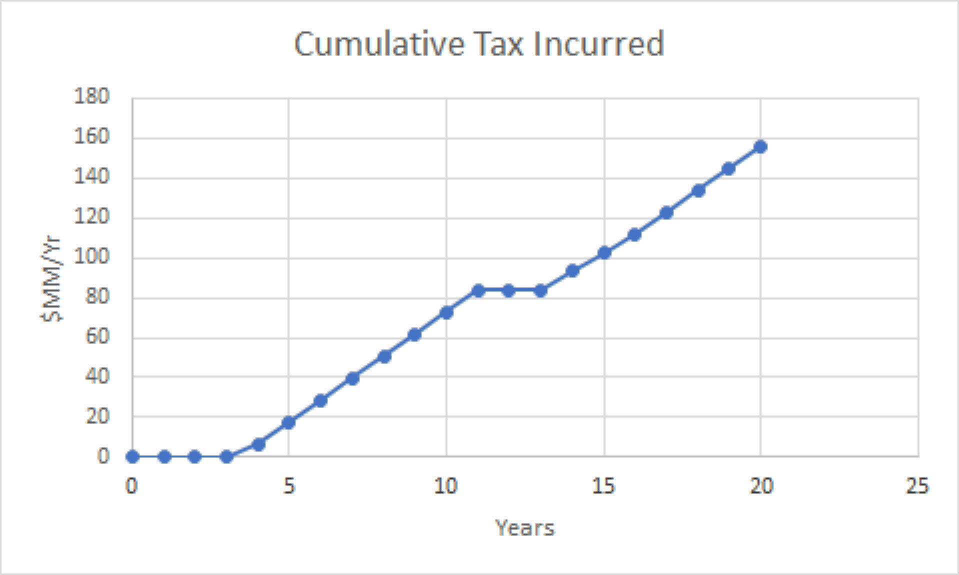
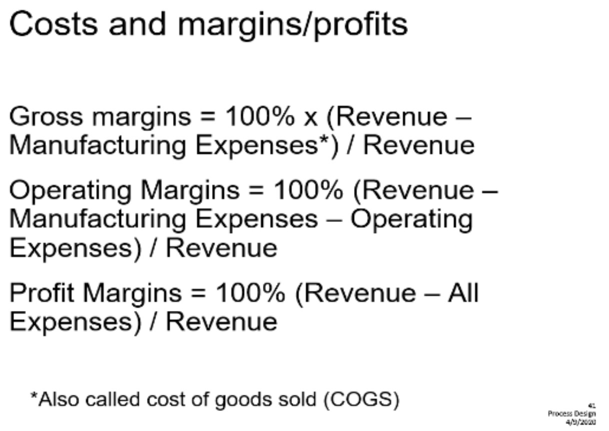


Figure 24: Graphical depiction of tax-rates in China's economic development zones

3.3.2 Margins

The gross, operating and profit margins were calculated by subtracting manufacturing expenses, operating expenses and all expenses respectively.



Costs and margins/profits

Gross margins = 100% x (Revenue – Manufacturing Expenses*) / Revenue

Operating Margins = 100% (Revenue – Manufacturing Expenses – Operating Expenses) / Revenue

Profit Margins = 100% (Revenue – All Expenses) / Revenue

*Also called cost of goods sold (COGS)

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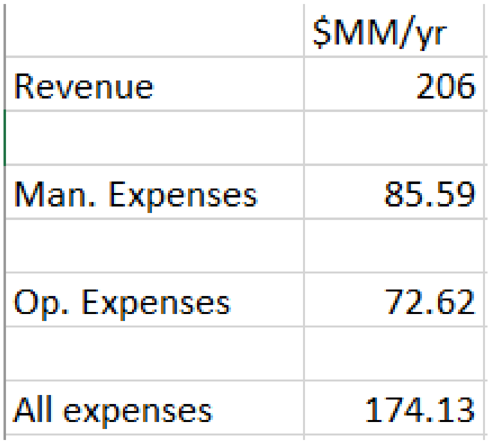
Figure 25: Methodology used to calculate margins



	$MM/yr
Revenue	206
Man. Expenses	85.59
Op. Expenses	72.62
All expenses	174.13

Table 12: The breakdown of the expenses

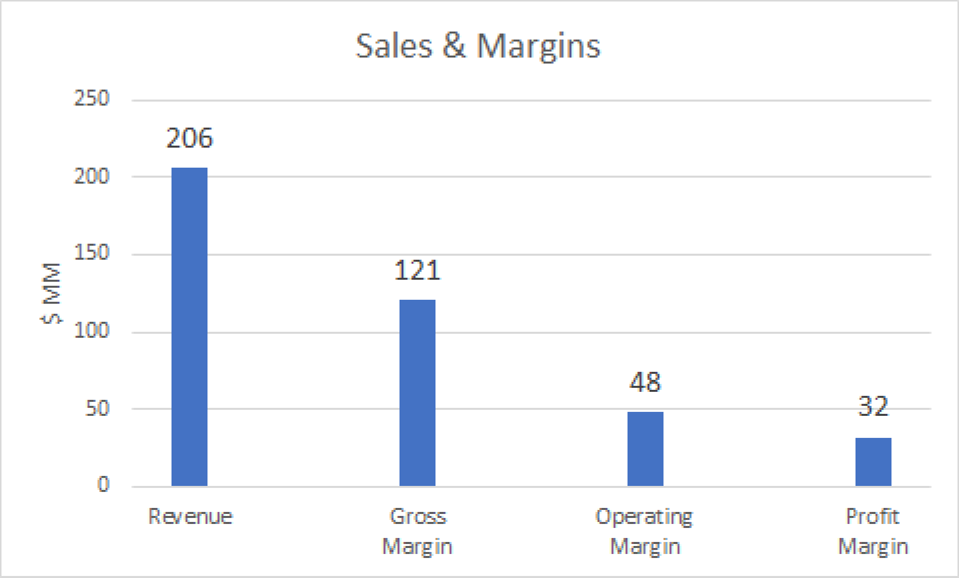


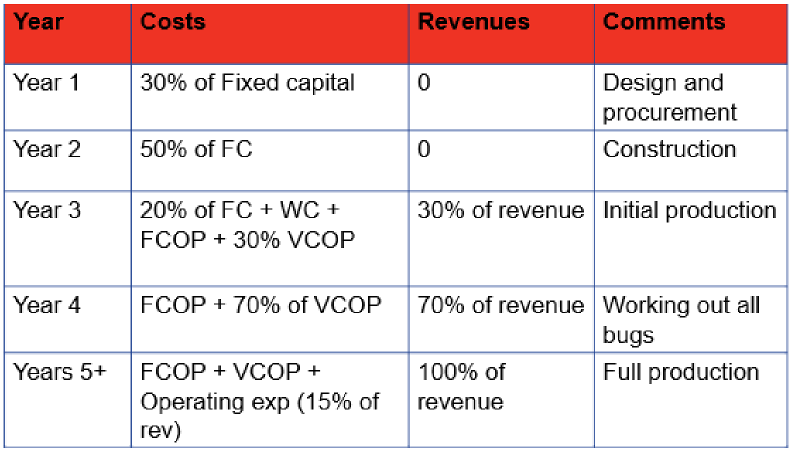
Figure 26: The sales and margins of the PMMA plant

3.3.3 Cash Flows:

The cash flows are determined using our total revenue after the sale of all PMMA products and Methyl Propionate by-products. The cumulative cash flow is determined using the compounded yearly revenues, the yearly operating costs, and the total fixed capital cost. Two models of cash flow are used to determine overall profitability. One accounts for depreciation, while one analyzes the cash flow in real time. The net present value function determines the cash flow each year in terms of the present value, using the weighted average cost of capital as the depreciation term.

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

Where n is the number of years following the project's startup. The net present value (NPV) is the compounded amounts of PV of all 20 years of the project’s lifetime combined. The startup schedule used to determine the running costs and cash flows over the lifetime of the project assumed full plant capacity by year 5.



Year	Costs	Revenues	Comments
Year 1	30% of Fixed capital	0	Design and procurement
Year 2	50% of FC	0	Construction
Year 3	20% of FC + WC + FCOP + 30% VCOP	30% of revenue	Initial production
Year 4	FCOP + 70% of VCOP	70% of revenue	Working out all bugs
Years 5+	FCOP + VCOP + Operating exp (15% of rev)	100% of revenue	Full production

Table 13: Startup Schedule

An analysis of the internal rate of return (IRR) of the proposed plant design predicts high profitability after 20 years of plant operation. A comparison of the IRR with the WACC reveals a difference of 14.3%, indicating large returns on the initial and running costs. Even after ten years, the return rate is found to be 13.4%, indicating that even with only 10 years of operation, the plant still remains largely profitable.

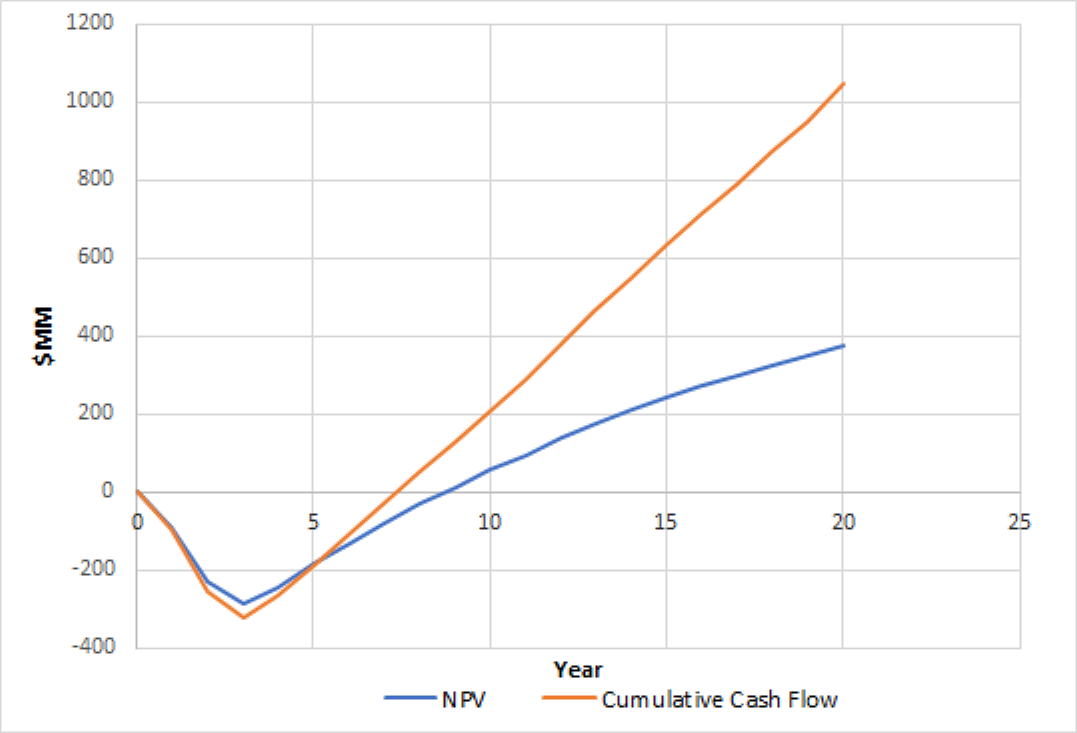


Figure 27: Cumulative Cash Flow and NPV

The break-even point is found to be at approximately 7 years after the initial construction.

The cumulative profit after 20 years is: $1039.13 MM

The cumulative NPV after 20 years is: $372 MM

4. Feasibility

4.1 Ethylene Scenario analysis

One of the scenarios analyzed was the alternative of using imported ethylene as a result of China's price instability[57]. China's domestic price of ethylene has been largely volatile due to start-up ethane crackers in Anhui province not doing as well as projected. The scenario analysis proposes importing ethylene from the United States instead of buying domestically under conditions where domestic ethylene prices are exorbitantly large or uncertain. The price of ethylene would be roughly 1100 $/ton, which is nearly double the previous local price of 565 $/ton. In the event of significant fluctuations in the local ethylene price, The OEAA group decided to analyze how to mitigate this issue in order to keep a reliable and consistent source of ethylene.

The main consequence of importing ethylene from the United States would be an increase in the yearly feedstock cost of production by $13 MM/yr compared to buying locally produced ethylene. This increase in the yearly cost of production would in turn decrease the yearly profits and cash flow by a great amount. The plant is still able to maintain its profitability and reach a cash flow break even point eight years into the investment as opposed to seven. Similarly, the net present value will remain in the negative for an extra year.

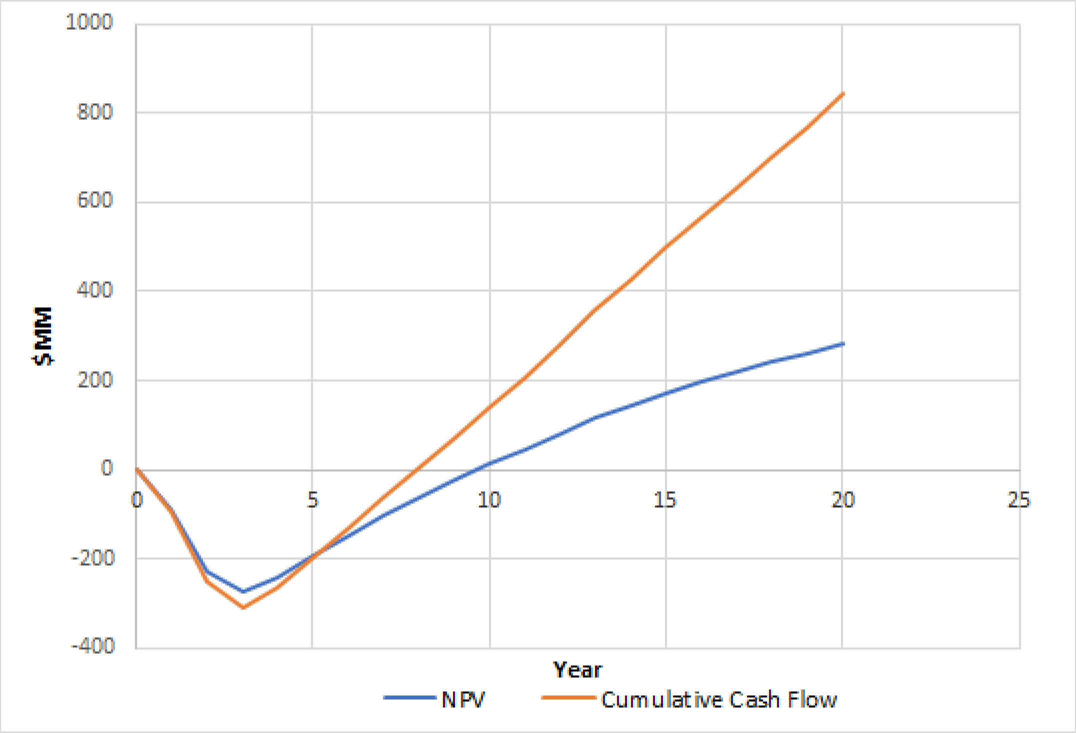


Figure 28: Cash flow and NPV assuming increased ethylene pricing

Despite the large increase in ethylene pricing, the plant still projects to maintain its profitability, albeit at a lower amount. In the event of a shift in ethylene procurement, the project projects reasonable profitability; this result indicates that the risk of this plant design is not particularly high, because the most volatile priced feedstock will not completely impede profitability at its maximum projected price. Overall, the plant is still able to recover relatively quickly if there had to be a shift in the procurement of ethylene, at double its original price.

4.2 Increased Production Scenario analysis

The second scenario analysis involves scaling up all input streams by 20% to effectively increase production by 20%. As described in the scoping section, China's increasing demand of PMMA could reasonably lead to a larger market. As such, plant scalability is a critical factor in determining plant design feasibility. An increase in domestic demand for PMMA could introduce the potential for increased profit in the design of a scaled-up plant. To accomodate for the scale-up, all feedstock and consumable materials such as methanol, ethylene, and pentane were introduced into the plant at an increased flow rate of 20%. Additionally, all plant unit operation sizes were increased by a factor of 20% by volume to produce similar conversions and purities as the original plant design. All other operation factors such as temperature, pressure, and similar variables were left the same. The changes resulted in what was roughly a 20% increase in plant throughput, with minimal changes in profit.

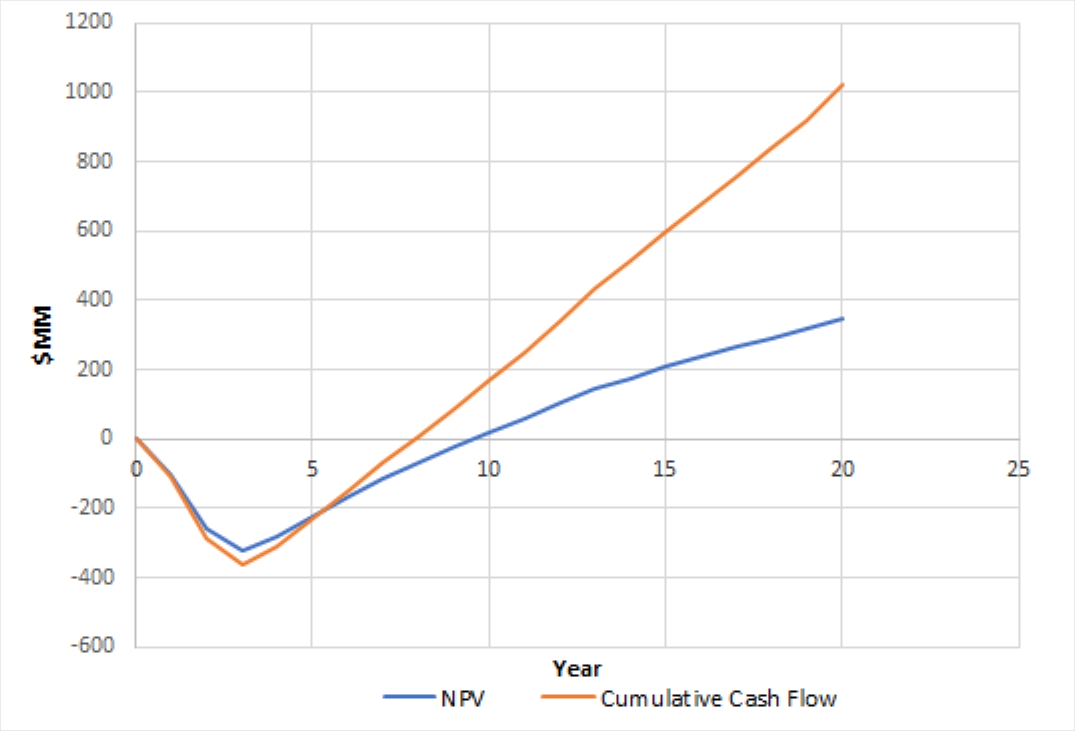


Figure 29: Cash Flow and NPV at increased plant throughput (20%)

The final CapEx of the scaled up plant is: $358.29 MM (12% higher)

The final OpEx of the scaled up plant is: $228.2 MM (21% higher)

The net Cash Flow of the scaled up plant is: $1020 MM (3% lower)

The NPV of the scaled up plant is: $345.12 MM (8% lower)

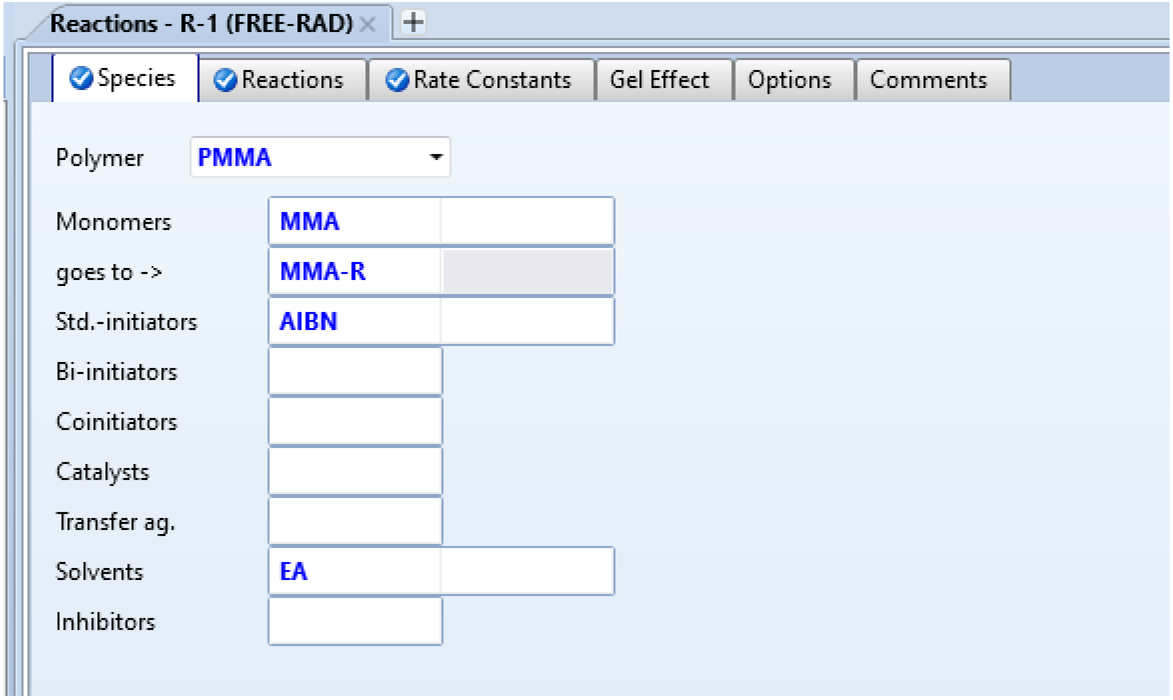
A cursory analysis of the original plant design with that of the scaled-up design shows that the profit of the scaled-up plant after 20 years is actually less. Although the profit decreases, the change is small. Nevertheless, the results can be used to show that scale-up of the proposed plant design is not feasible, and that the plant capacity is already at its maximum given the current design. One possible method of increasing plant throughput without decreasing profitability would be to introduce parallel unit operations in place of increasing unit dimensions, but at a significantly larger increase in throughput than just 20%. Another possible method is to revamp the entire separation scheme used in order to achieve the same separation but with a lower solvent use (or higher recovery) to lower Opex. Additionally, the FBR (which accounts for 76% of the total installed equipment cost for the entire plant) can be redesigned to be much smaller if a lower conversion MP is acceptable (then recycling of MP would need to be implemented). Thus, a scaled-up design of the current plant is unfeasible without drastic design changes which might only help minimally even if done, which suggests that the maximum profit to be gained from the proposed plant design lies somewhere near the current plant output.

5. Conclusion

The OEAA group determined through preliminary investigation that the production of PMMA as a product for sale is a technically and economically feasible project. The PMMA plant to be located in Hefei, Anhui in China was determined to be economically feasible through market indicators suggesting that overall regional growth was healthy and steadily rising at a CAGR of 9.1% for beads in the global market; the total market volume was determined to be approximately 4.8 billion dollars. Additionally, the same sources suggested that the largest market volume for the PMMA market was located in the Asia-Pacific region, thus justifying the decision to locate the plant in China. Furthermore, the technical feasibility was justified based on the selected PMMA production method's prevalence in industry, alongside its constituting feedstock's accessibility in the chosen region as well as other factors. The anticipated plant capacity was determined to be 50,000 tonnes to be sold at a price of 3000 \$/tonne, totalling to a \$150 MM SOM. Moving forward, the OEAA group plans to begin the design phase of the proposed plant, and to begin selection of particular feedstock sources and catalyst materials to be used in the production of our PMMA beads. After investigation, team OEAA produced a feasible design for the proposed plant using Aspen Plus V10 at a final throughput of 58,482 tonnes/Yr. The resulting plant was determined to net a total profit of \$1.05 Bn and a net present value (NPV) of \$376.82 MM. A feasibility analysis examined the potential for a price increase on the most volatile feedstock and indicated that the plant remains reasonably profitable, even at significantly increased operating costs. Additionally, potential for an increase in plant throughput via plant scaleup was shown to be infeasible due to a decrease in overall profit at the proposed throughput increase. This result conclusively showed that the current plant design proposal is already operating somewhere near the maximum possible profit.

6. Appendices:

Appendix A: Design Phase



Polymer PMMA

Monomers MMA

goes to -> MMA-R

Std.-initiators AIBN

Bi-initiators

Coinitiators

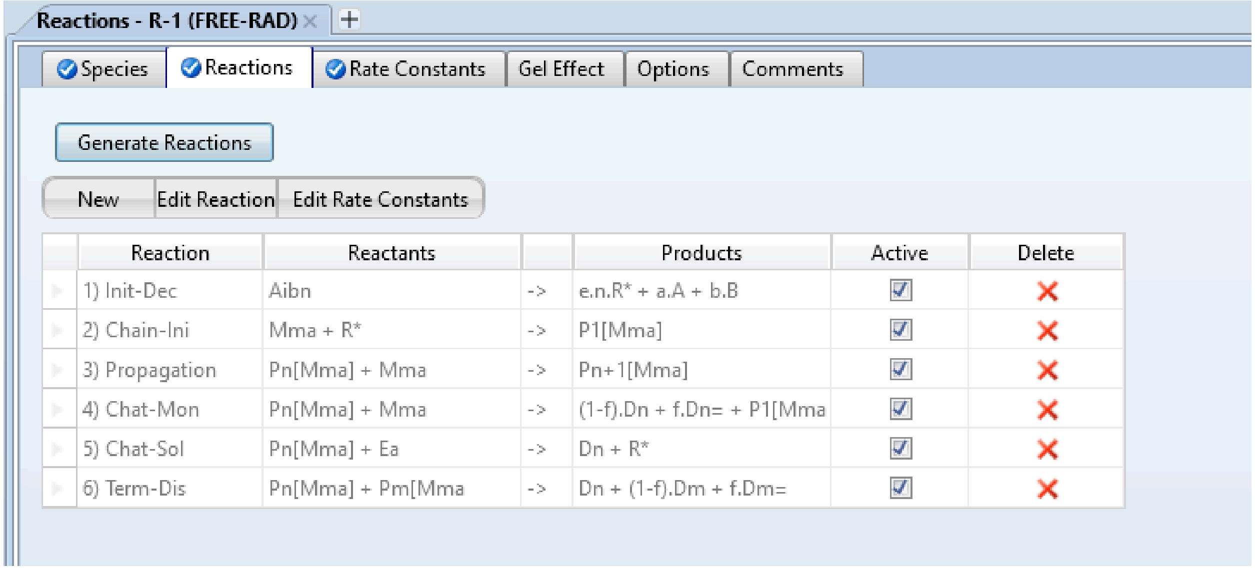
Catalysts

Transfer ag.

Solvents EA

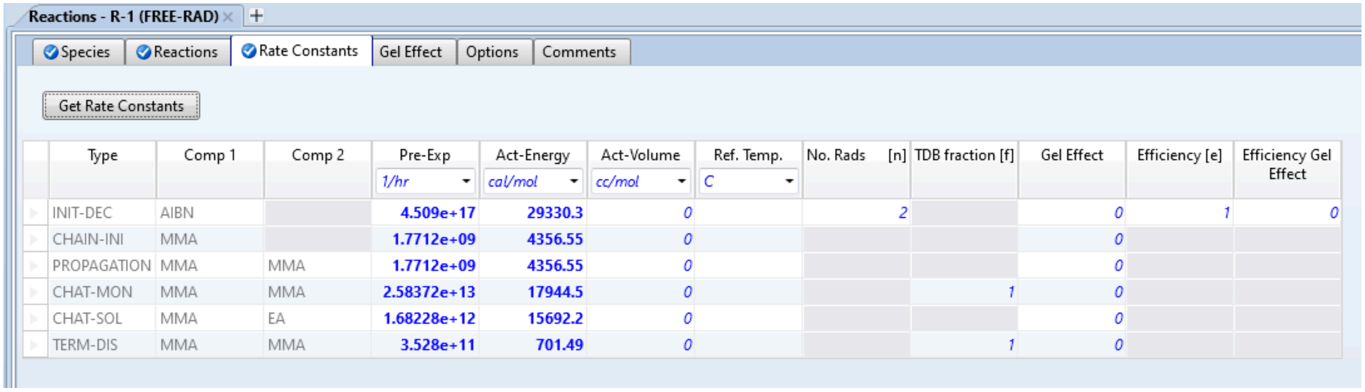
Inhibitors

Figure A1: Species involved in the polymerization reaction



Reaction	Reactants		Products	Active	Delete
1) Init-Dec	Aibn	->	e.n.R* + a.A + b.B	☑	✗
2) Chain-Ini	Mma + R*	->	P1[Mma]	☑	✗
3) Propagation	Pn[Mma] + Mma	->	Pn+1[Mma]	☑	✗
4) Chat-Mon	Pn[Mma] + Mma	->	(1-f).Dn + f.Dn= + P1[Mma	☑	✗
5) Chat-Sol	Pn[Mma] + Ea	->	Dn + R*	☑	✗
6) Term-Dis	Pn[Mma] + Pm[Mma	->	Dn + (1-f).Dm + f.Dm=	☑	✗

Figures A2: Reaction stoichiometry of polymerization steps



Type	Comp 1	Comp 2	Pre-Exp 1/hr	Act-Energy cal/mol	Act-Volume cc/mol	Ref. Temp. C	No. Rads [n]	TDB fraction [f]	Gel Effect	Efficiency [e]	Efficiency Gel Effect
INIT-DEC	AIBN		4.509e+17	29330.3	0		2		0	1	0
CHAIN-INI	MMA		1.7712e+09	4356.55	0				0		
PROPAGATION	MMA	MMA	1.7712e+09	4356.55	0				0		
CHAT-MON	MMA	MMA	2.58372e+13	17944.5	0			1	0		
CHAT-SOL	MMA	EA	1.68228e+12	15692.2	0				0		
TERM-DIS	MMA	MMA	3.528e+11	701.49	0			1	0		

Figure A3: Rate constants of individual polymerization steps

Utility Type and Units	Unit Op Name	Rate	Equipment
Electricity (kW)	EXTRUDERS (all)	70.3	Extruder
	PUMP1	32.3	Centrifugal Pump
	PUMP2	6.1	Centrifugal Pump
	PUMP3	-3.0	Centrifugal Pump
	DISTILL5-reflux pump	4.1	Centrifugal Pump
	DISTILL4-reflux pump	8.3	Centrifugal Pump
	DISTILL3-reflux pump	20.7	Centrifugal Pump
	DISTILL2-reflux pump	24.9	Centrifugal Pump
	DISTILL1-reflux pump	8.3	Centrifugal Pump
	MCOMPRES	2487.2	Centrifugal

			Compressor
	COMPRESS	684.1	Centrifugal Compressor
	EXPANDER	-852.2	Centrifugal Expander
	EXPANDR2	-337.3	Centrifugal Expander
HP Steam (klb/hr)	HEATER1	16.6	DHE HeatX
	HEATER3	3.5	DHE HeatX
MP Steam (klb/hr)	DISTILL1-reb	15.6	U-Tube HeatX
	DISTILL3-reb	37.5	U-Tube HeatX
	DISTILL4-reb	8.1	U-Tube HeatX
	DISTILL2-reb	36.6	U-Tube HeatX
	DISTILL5-reb	4.6	U-Tube HeatX
	HEATER2	16.7	DHE HeatX
Cooling Water (MMGal/hr	DISTILL3-cond	0.2	DHE HeatX
	CHILLER3	0.04	DHE HeatX
	DISTILL4-cond	0.05	DHE HeatX
	CHILLER4	0.03	DHE HeatX
	DISTILL5-cond	0.02	DHE HeatX
NG (kg/hr)	HEATER-4	218.8	Furnace
Refrigeration (klb/hr of Freon-12)	DISTILL1-cond	103.2	DHE HeatX
	DISTILL2-cond	397.5	DHE HeatX
	CHILLER1	286.8	DHE HeatX
	CHILLER2	66.5	DHE HeatX

Table A1: Detailed Utilities Information

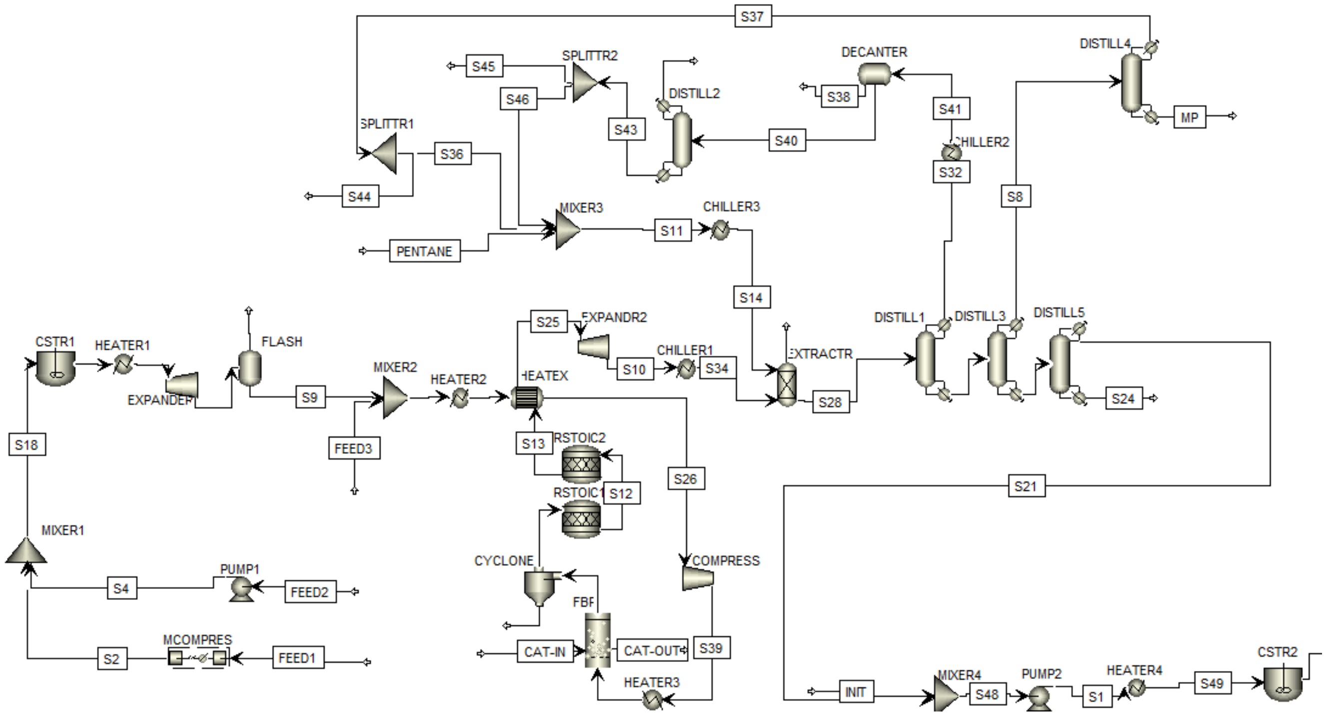


Figure A4.a: Flowsheet of final proposed design process (excluding extruders)

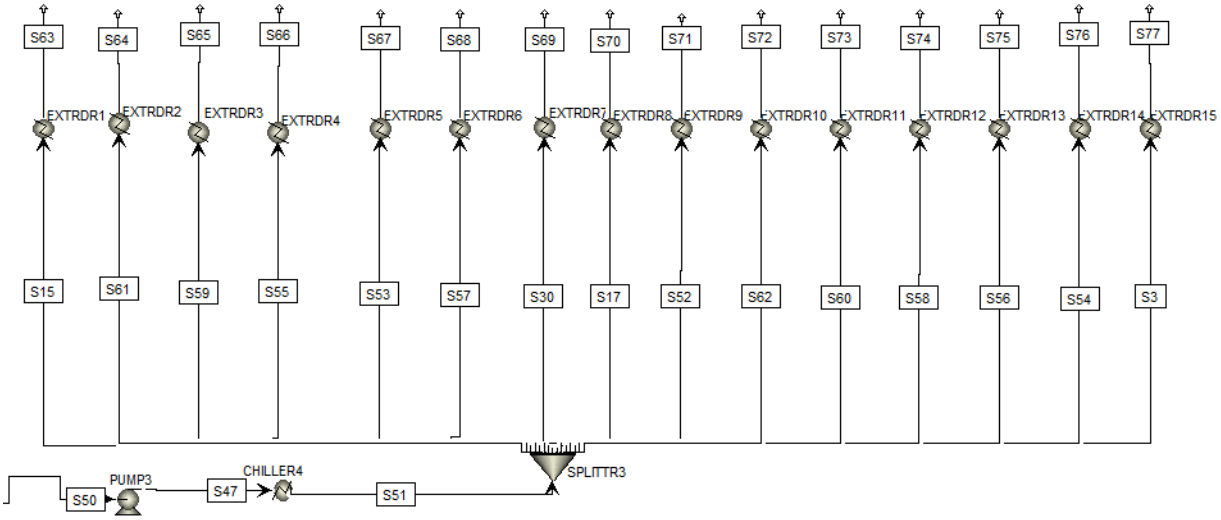
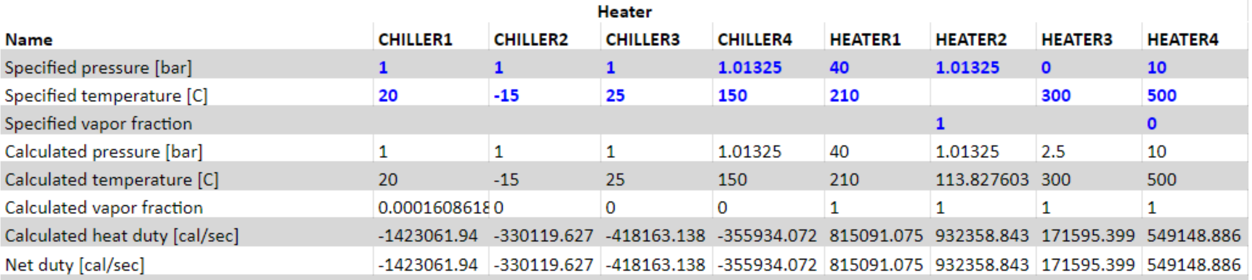
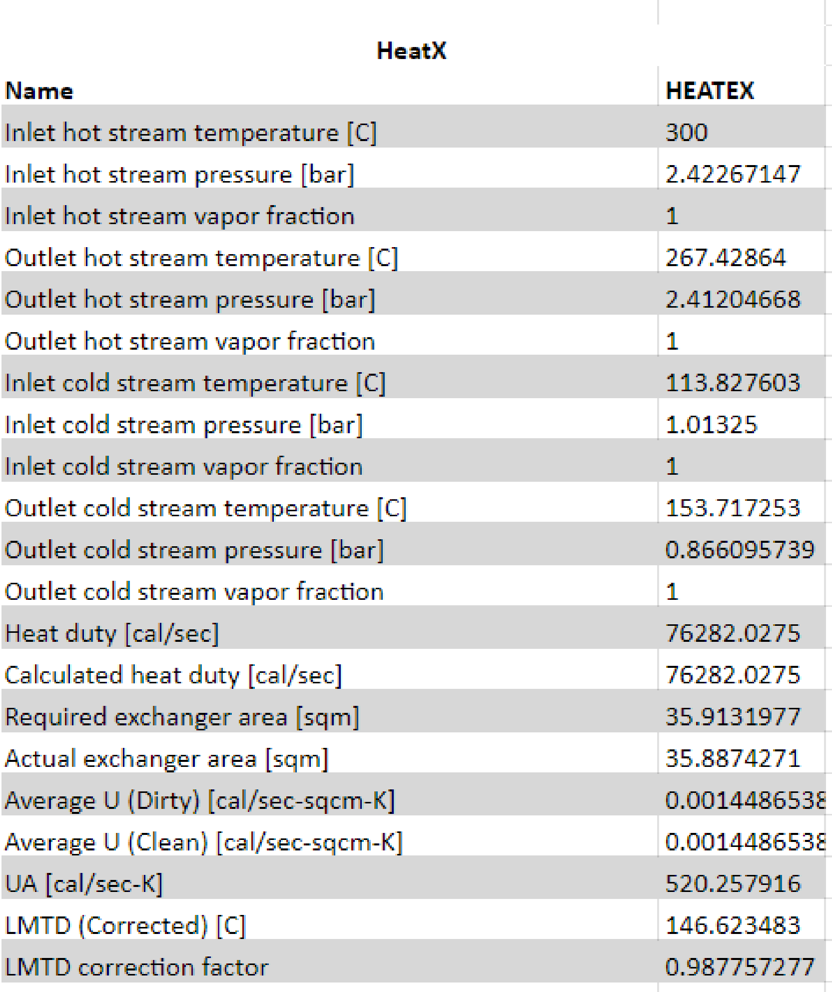


Figure A4.b: Flowsheet of final proposed design process (extrusion)



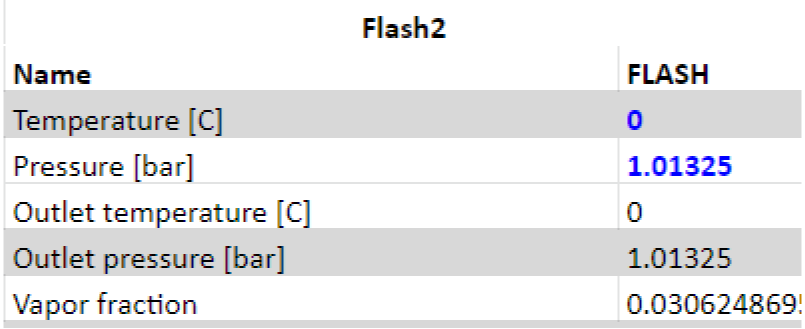
Name	CHILLER1	CHILLER2	CHILLER3	CHILLER4	HEATER1	HEATER2	HEATER3	HEATER4
			Heater					
Specified pressure [bar]	**1**	**1**	**1**	**1.01325**	**40**	**1.01325**	**0**	**10**
Specified temperature [C]	**20**	**-15**	**25**	**150**	**210**		**300**	**500**
Specified vapor fraction						**1**		**0**
Calculated pressure [bar]	1	1	1	1.01325	40	1.01325	2.5	10
Calculated temperature [C]	20	-15	25	150	210	113.827603	300	500
Calculated vapor fraction	0.0001608618	0	0	0	1	1	1	1
Calculated heat duty [cal/sec]	-1423061.94	-330119.627	-418163.138	-355934.072	815091.075	932358.843	171595.399	549148.886
Net duty [cal/sec]	-1423061.94	-330119.627	-418163.138	-355934.072	815091.075	932358.843	171595.399	549148.886

Figure A5: Heater and Chiller design specifications



HeatX	
Name	**HEATEX**
Inlet hot stream temperature [C]	300
Inlet hot stream pressure [bar]	2.42267147
Inlet hot stream vapor fraction	1
Outlet hot stream temperature [C]	267.42864
Outlet hot stream pressure [bar]	2.41204668
Outlet hot stream vapor fraction	1
Inlet cold stream temperature [C]	113.827603
Inlet cold stream pressure [bar]	1.01325
Inlet cold stream vapor fraction	1
Outlet cold stream temperature [C]	153.717253
Outlet cold stream pressure [bar]	0.866095739
Outlet cold stream vapor fraction	1
Heat duty [cal/sec]	76282.0275
Calculated heat duty [cal/sec]	76282.0275
Required exchanger area [sqm]	35.9131977
Actual exchanger area [sqm]	35.8874271
Average U (Dirty) [cal/sec-sqcm-K]	0.0014486538
Average U (Clean) [cal/sec-sqcm-K]	0.0014486538
UA [cal/sec-K]	520.257916
LMTD (Corrected) [C]	146.623483
LMTD correction factor	0.987757277

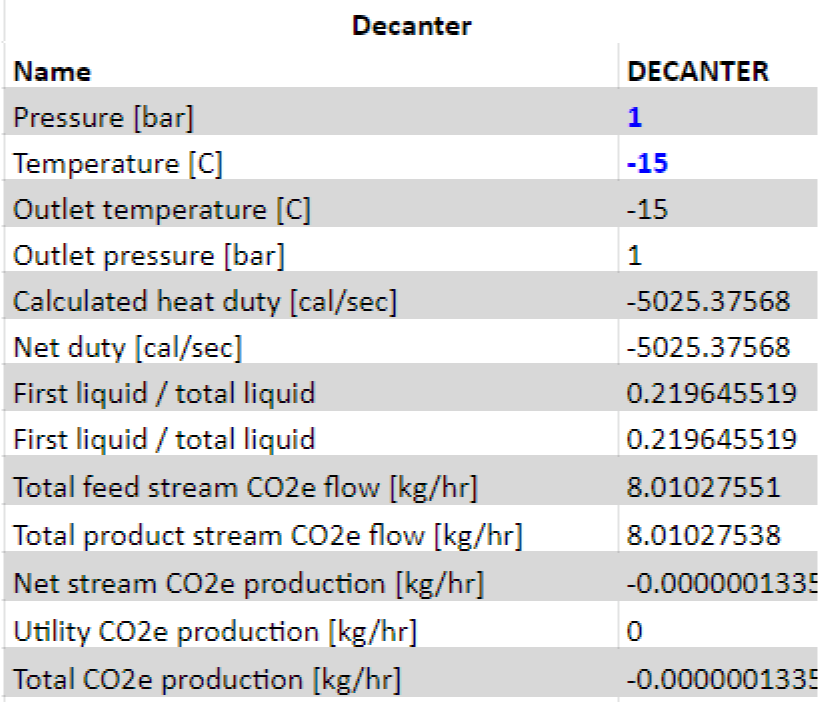
Figure A6: Heat Exchanger Design Specifications



Flash2

Name	**FLASH**
Temperature [C]	**0**
Pressure [bar]	**1.01325**
Outlet temperature [C]	0
Outlet pressure [bar]	1.01325
Vapor fraction	0.030624869

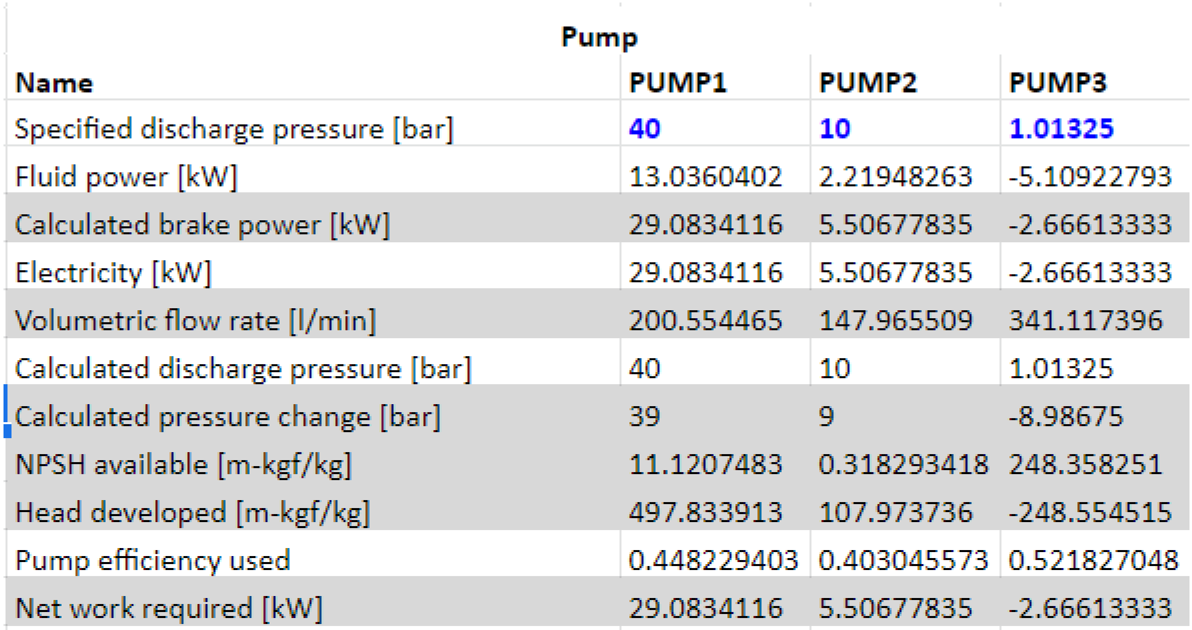
Figure A7: Flash Unit operation design specifications



Decanter

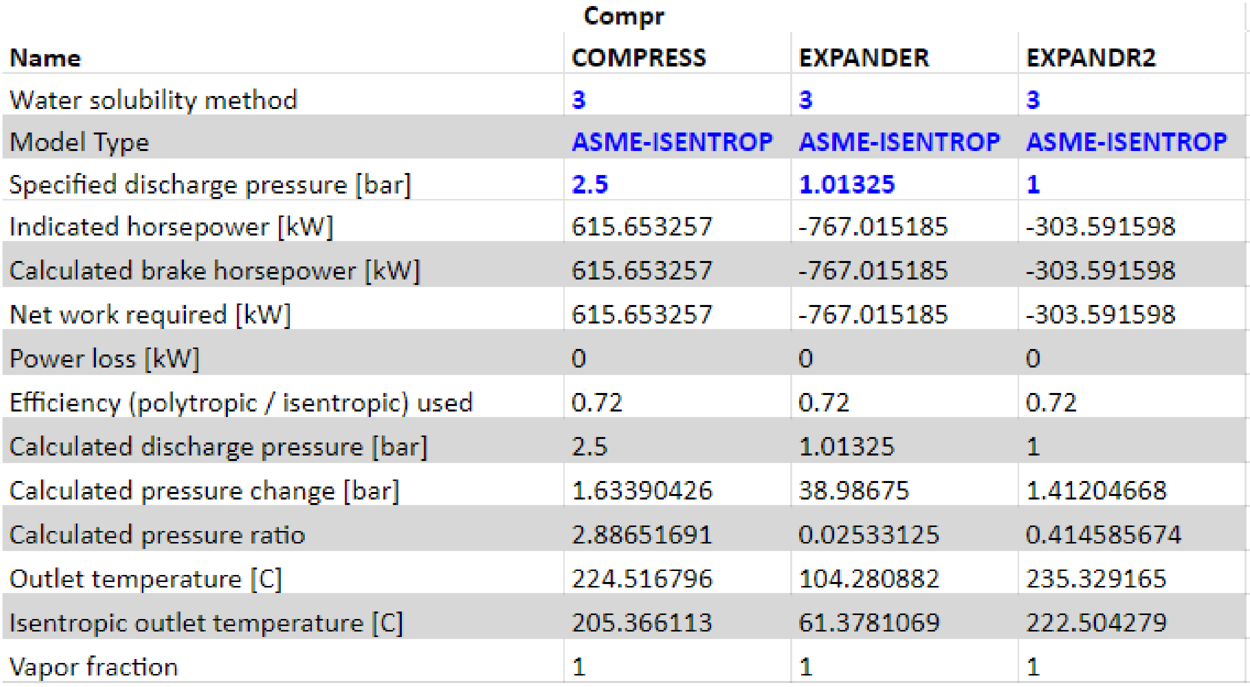
Name	**DECANTER**
Pressure [bar]	**1**
Temperature [C]	**-15**
Outlet temperature [C]	-15
Outlet pressure [bar]	1
Calculated heat duty [cal/sec]	-5025.37568
Net duty [cal/sec]	-5025.37568
First liquid / total liquid	0.219645519
First liquid / total liquid	0.219645519
Total feed stream CO2e flow [kg/hr]	8.01027551
Total product stream CO2e flow [kg/hr]	8.01027538
Net stream CO2e production [kg/hr]	-0.000000133
Utility CO2e production [kg/hr]	0
Total CO2e production [kg/hr]	-0.000000133

Figure A8: Decanter design specifications



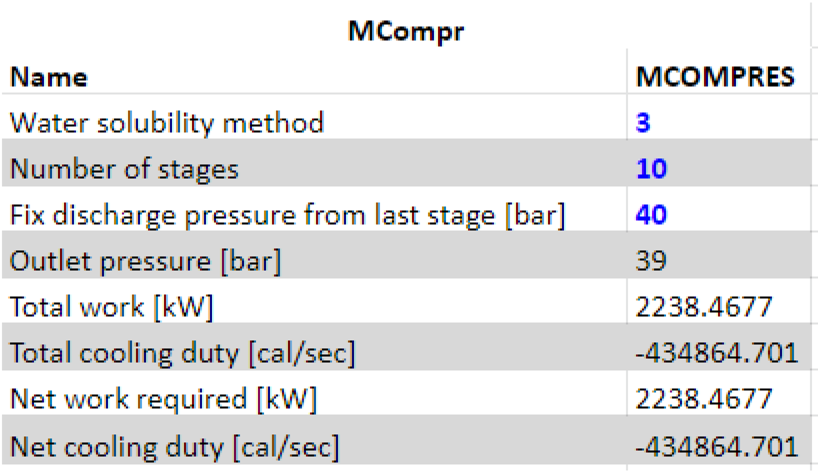
	Pump		
Name	**PUMP1**	**PUMP2**	**PUMP3**
Specified discharge pressure [bar]	**40**	**10**	**1.01325**
Fluid power [kW]	13.0360402	2.21948263	-5.10922793
Calculated brake power [kW]	29.0834116	5.50677835	-2.66613333
Electricity [kW]	29.0834116	5.50677835	-2.66613333
Volumetric flow rate [l/min]	200.554465	147.965509	341.117396
Calculated discharge pressure [bar]	40	10	1.01325
Calculated pressure change [bar]	39	9	-8.98675
NPSH available [m-kgf/kg]	11.1207483	0.318293418	248.358251
Head developed [m-kgf/kg]	497.833913	107.973736	-248.554515
Pump efficiency used	0.448229403	0.403045573	0.521827048
Net work required [kW]	29.0834116	5.50677835	-2.66613333

Figure A9: All Pump design specifications



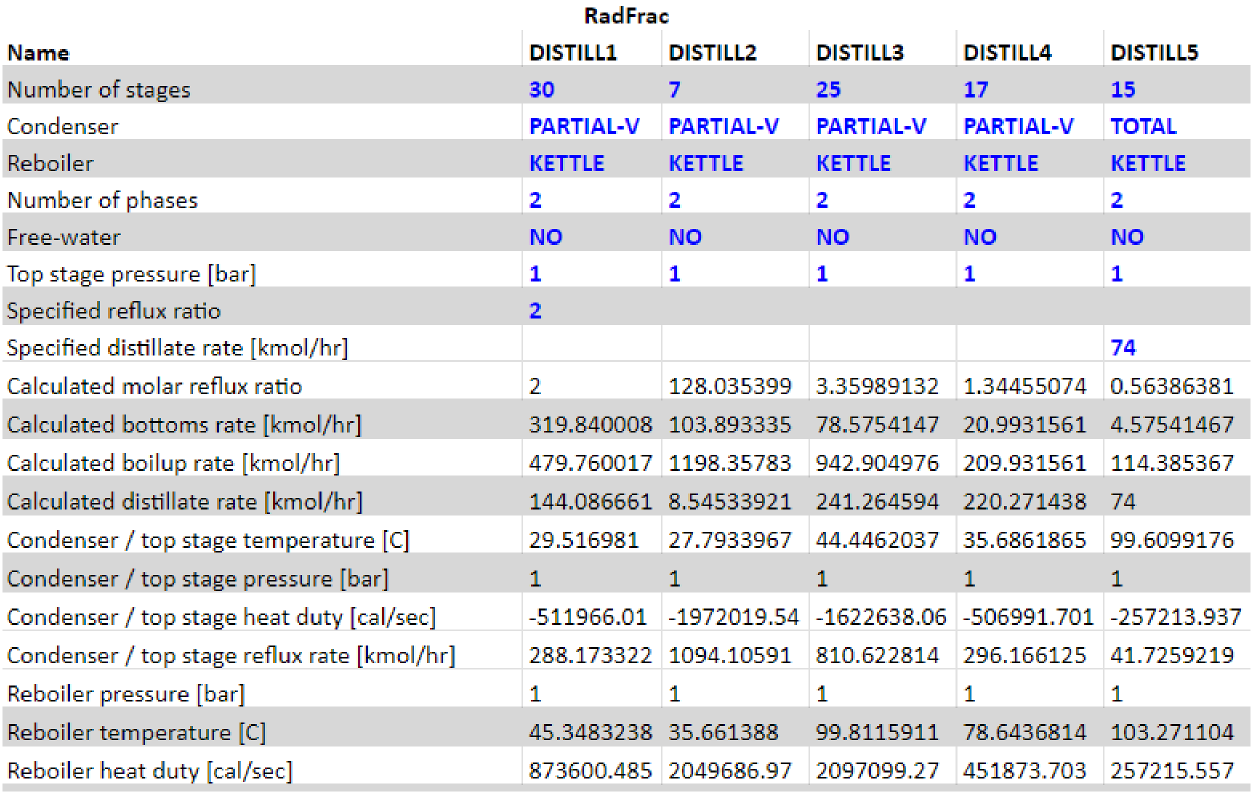
	Compr		
Name	**COMPRESS**	**EXPANDER**	**EXPANDR2**
Water solubility method	**3**	**3**	**3**
Model Type	**ASME-ISENTROP**	**ASME-ISENTROP**	**ASME-ISENTROP**
Specified discharge pressure [bar]	**2.5**	**1.01325**	**1**
Indicated horsepower [kW]	615.653257	-767.015185	-303.591598
Calculated brake horsepower [kW]	615.653257	-767.015185	-303.591598
Net work required [kW]	615.653257	-767.015185	-303.591598
Power loss [kW]	0	0	0
Efficiency (polytropic / isentropic) used	0.72	0.72	0.72
Calculated discharge pressure [bar]	2.5	1.01325	1
Calculated pressure change [bar]	1.63390426	38.98675	1.41204668
Calculated pressure ratio	2.88651691	0.02533125	0.414585674
Outlet temperature [C]	224.516796	104.280882	235.329165
Isentropic outlet temperature [C]	205.366113	61.3781069	222.504279
Vapor fraction	1	1	1

Figure A10: All Compressor design specifications



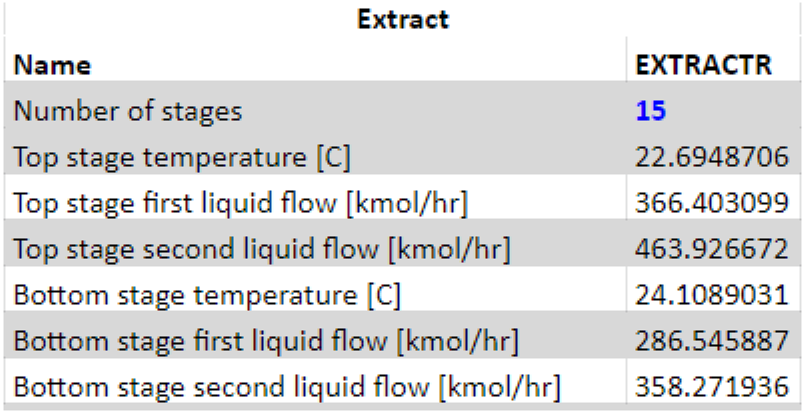
MCompr	
Name	MCOMPRES
Water solubility method	3
Number of stages	10
Fix discharge pressure from last stage [bar]	40
Outlet pressure [bar]	39
Total work [kW]	2238.4677
Total cooling duty [cal/sec]	-434864.701
Net work required [kW]	2238.4677
Net cooling duty [cal/sec]	-434864.701

Figure A11: Multi-stage Cooling Compressor design specifications



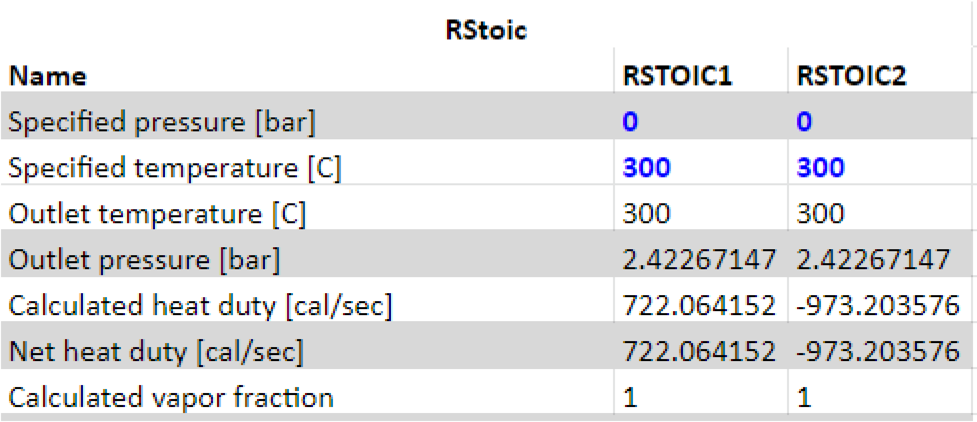
RadFrac					
Name	DISTILL1	DISTILL2	DISTILL3	DISTILL4	DISTILL5
Number of stages	30	7	25	17	15
Condenser	PARTIAL-V	PARTIAL-V	PARTIAL-V	PARTIAL-V	TOTAL
Reboiler	KETTLE	KETTLE	KETTLE	KETTLE	KETTLE
Number of phases	2	2	2	2	2
Free-water	NO	NO	NO	NO	NO
Top stage pressure [bar]	1	1	1	1	1
Specified reflux ratio	2				
Specified distillate rate [kmol/hr]					74
Calculated molar reflux ratio	2	128.035399	3.35989132	1.34455074	0.56386381
Calculated bottoms rate [kmol/hr]	319.840008	103.893335	78.5754147	20.9931561	4.57541467
Calculated boilup rate [kmol/hr]	479.760017	1198.35783	942.904976	209.931561	114.385367
Calculated distillate rate [kmol/hr]	144.086661	8.54533921	241.264594	220.271438	74
Condenser / top stage temperature [C]	29.516981	27.7933967	44.4462037	35.6861865	99.6099176
Condenser / top stage pressure [bar]	1	1	1	1	1
Condenser / top stage heat duty [cal/sec]	-511966.01	-1972019.54	-1622638.06	-506991.701	-257213.937
Condenser / top stage reflux rate [kmol/hr]	288.173322	1094.10591	810.622814	296.166125	41.7259219
Reboiler pressure [bar]	1	1	1	1	1
Reboiler temperature [C]	45.3483238	35.661388	99.8115911	78.6436814	103.271104
Reboiler heat duty [cal/sec]	873600.485	2049686.97	2097099.27	451873.703	257215.557

Figure A12: All Distillation Column design specifications



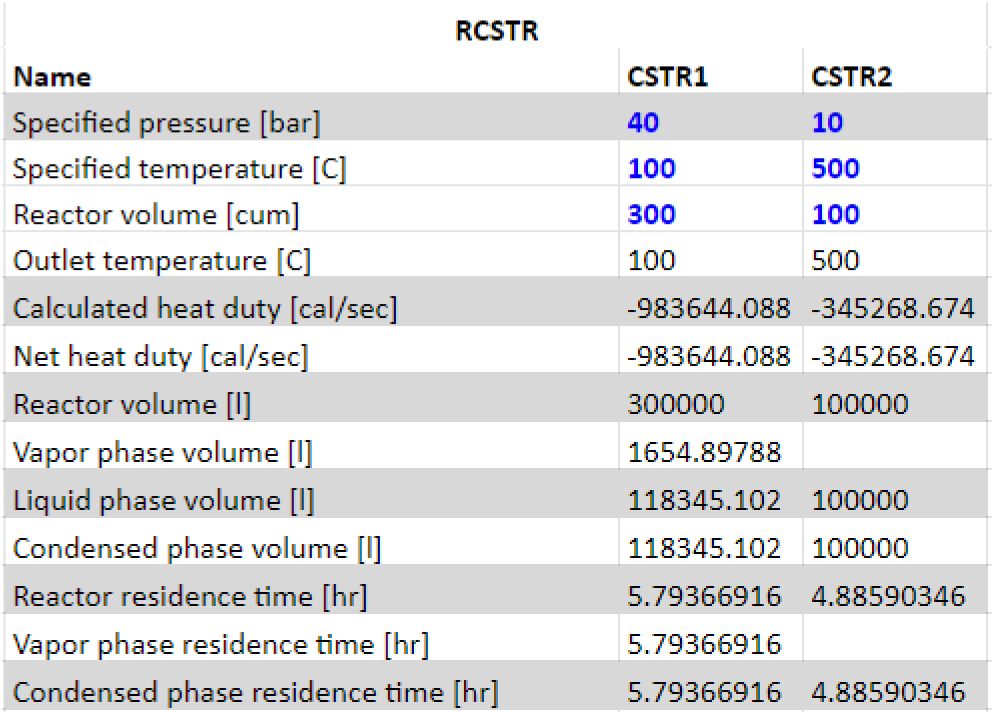
Extract	
Name	**EXTRACTR**
Number of stages	**15**
Top stage temperature [C]	22.6948706
Top stage first liquid flow [kmol/hr]	366.403099
Top stage second liquid flow [kmol/hr]	463.926672
Bottom stage temperature [C]	24.1089031
Bottom stage first liquid flow [kmol/hr]	286.545887
Bottom stage second liquid flow [kmol/hr]	358.271936

Figure A13: Extractor design specifications



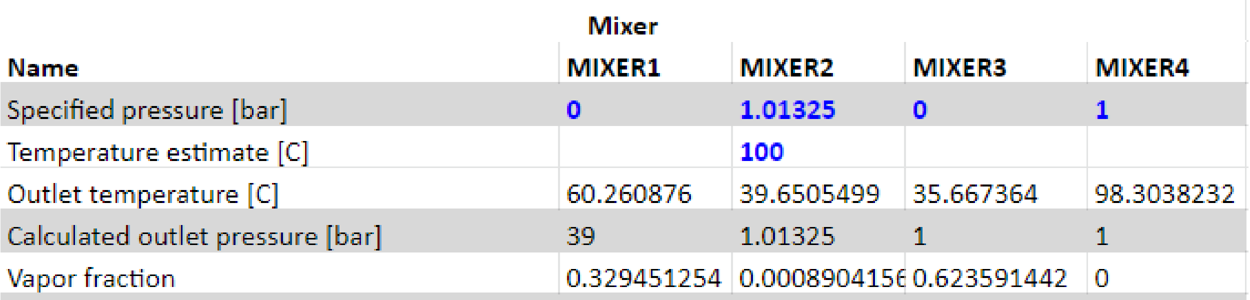
RStoic		
Name	**RSTOIC1**	**RSTOIC2**
Specified pressure [bar]	**0**	**0**
Specified temperature [C]	**300**	**300**
Outlet temperature [C]	300	300
Outlet pressure [bar]	2.42267147	2.42267147
Calculated heat duty [cal/sec]	722.064152	-973.203576
Net heat duty [cal/sec]	722.064152	-973.203576
Calculated vapor fraction	1	1

Figure A14: All Rstoic units design specifications



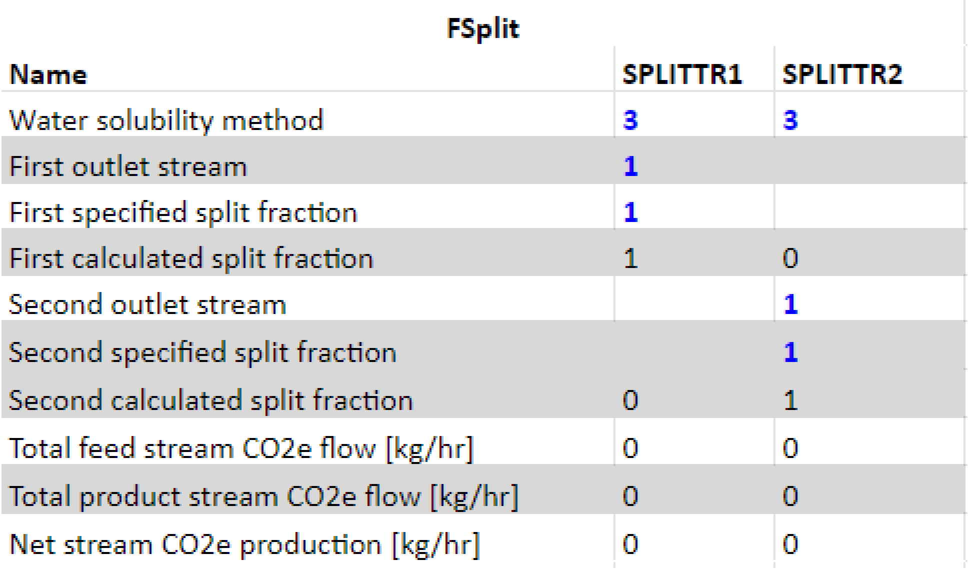
RCSTR		
Name	**CSTR1**	**CSTR2**
Specified pressure [bar]	**40**	**10**
Specified temperature [C]	**100**	**500**
Reactor volume [cum]	**300**	**100**
Outlet temperature [C]	100	500
Calculated heat duty [cal/sec]	-983644.088	-345268.674
Net heat duty [cal/sec]	-983644.088	-345268.674
Reactor volume [l]	300000	100000
Vapor phase volume [l]	1654.89788	
Liquid phase volume [l]	118345.102	100000
Condensed phase volume [l]	118345.102	100000
Reactor residence time [hr]	5.79366916	4.88590346
Vapor phase residence time [hr]	5.79366916	
Condensed phase residence time [hr]	5.79366916	4.88590346

Figure A15: All CSTR design specifications



Mixer				
Name	**MIXER1**	**MIXER2**	**MIXER3**	**MIXER4**
Specified pressure [bar]	**0**	**1.01325**	**0**	**1**
Temperature estimate [C]		**100**		
Outlet temperature [C]	60.260876	39.6505499	35.667364	98.3038232
Calculated outlet pressure [bar]	39	1.01325	1	1
Vapor fraction	0.329451254	0.0008904156	0.623591442	0

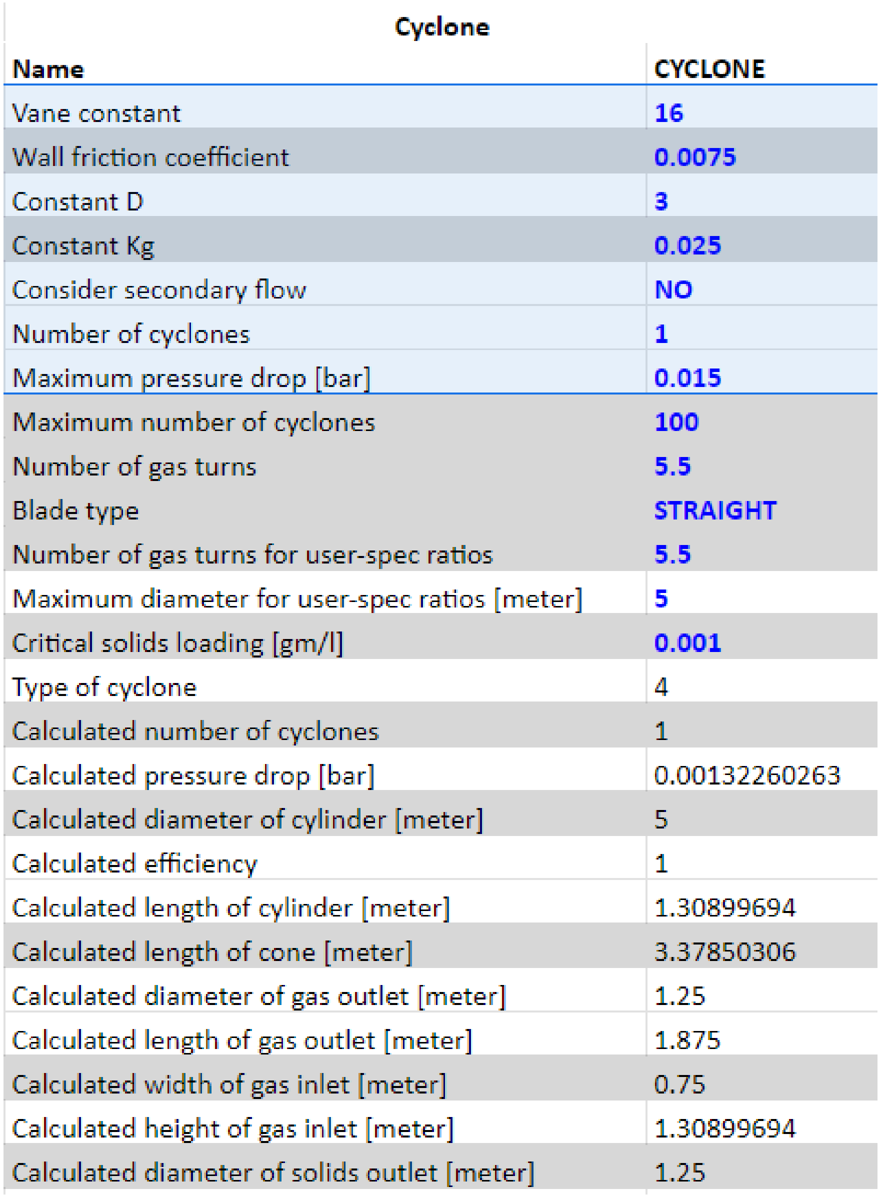
Figure A16: All Mixer design specifications



FSplit

Name	SPLITTR1	SPLITTR2
Water solubility method	3	3
First outlet stream	1	
First specified split fraction	1	
First calculated split fraction	1	0
Second outlet stream		1
Second specified split fraction		1
Second calculated split fraction	0	1
Total feed stream CO2e flow [kg/hr]	0	0
Total product stream CO2e flow [kg/hr]	0	0
Net stream CO2e production [kg/hr]	0	0

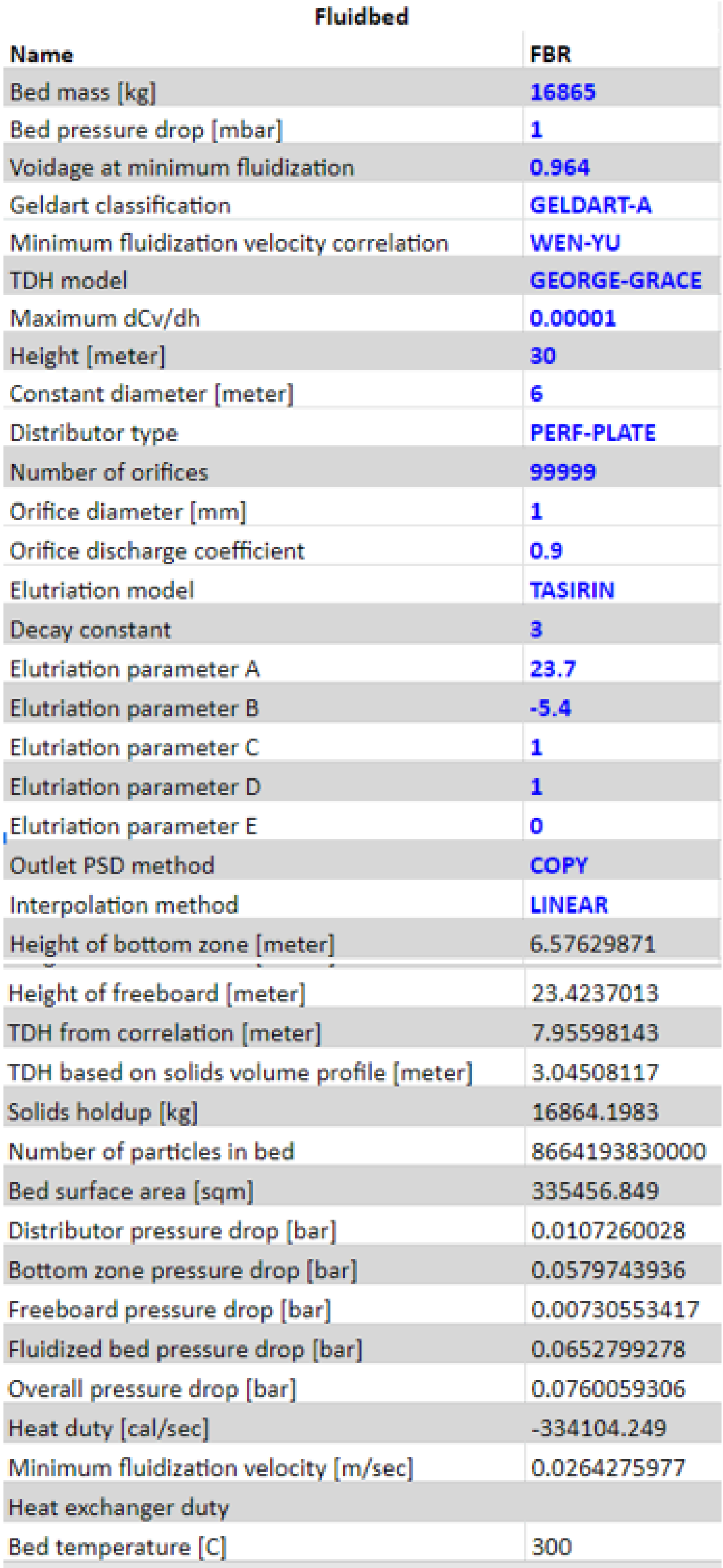
Figure A17: All Splitter Design specifications



Cyclone

Name	CYCLONE
Vane constant	16
Wall friction coefficient	0.0075
Constant D	3
Constant Kg	0.025
Consider secondary flow	NO
Number of cyclones	1
Maximum pressure drop [bar]	0.015
Maximum number of cyclones	100
Number of gas turns	5.5
Blade type	STRAIGHT
Number of gas turns for user-spec ratios	5.5
Maximum diameter for user-spec ratios [meter]	5
Critical solids loading [gm/l]	0.001
Type of cyclone	4
Calculated number of cyclones	1
Calculated pressure drop [bar]	0.00132260263
Calculated diameter of cylinder [meter]	5
Calculated efficiency	1
Calculated length of cylinder [meter]	1.30899694
Calculated length of cone [meter]	3.37850306
Calculated diameter of gas outlet [meter]	1.25
Calculated length of gas outlet [meter]	1.875
Calculated width of gas inlet [meter]	0.75
Calculated height of gas inlet [meter]	1.30899694
Calculated diameter of solids outlet [meter]	1.25

Figure A18: Cyclone design specifications



Fluidbed

Name	FBR
Bed mass [kg]	16865
Bed pressure drop [mbar]	1
Voidage at minimum fluidization	0.964
Geldart classification	GELDART-A
Minimum fluidization velocity correlation	WEN-YU
TDH model	GEORGE-GRACE
Maximum dCv/dh	0.00001
Height [meter]	30
Constant diameter [meter]	6
Distributor type	PERF-PLATE
Number of orifices	99999
Orifice diameter [mm]	1
Orifice discharge coefficient	0.9
Elutriation model	TASIRIN
Decay constant	3
Elutriation parameter A	23.7
Elutriation parameter B	-5.4
Elutriation parameter C	1
Elutriation parameter D	1
Elutriation parameter E	0
Outlet PSD method	COPY
Interpolation method	LINEAR
Height of bottom zone [meter]	6.57629871
Height of freeboard [meter]	23.4237013
TDH from correlation [meter]	7.95598143
TDH based on solids volume profile [meter]	3.04508117
Solids holdup [kg]	16864.1983
Number of particles in bed	8664193830000
Bed surface area [sqm]	335456.849
Distributor pressure drop [bar]	0.0107260028
Bottom zone pressure drop [bar]	0.0579743936
Freeboard pressure drop [bar]	0.00730553417
Fluidized bed pressure drop [bar]	0.0652799278
Overall pressure drop [bar]	0.0760059306
Heat duty [cal/sec]	-334104.249
Minimum fluidization velocity [m/sec]	0.0264275977
Heat exchanger duty	
Bed temperature [C]	300

Figure A19: Fluidized Bed Reactor design specifications

Appendix B: Economics Phase

Unit Op Name in Aspen	Method	C_e ($ MM)	Install Factor	C_i ($ MM)
FBR	[78],[79],[80]	48	3	143
CSTR1	1+2	4	3	11
MCOMPRES	1	3	2.5	7
EXPANDER	1	2	2.5	4
COMPRESS	1	2	2.5	4
CSTR2	1+2	1	3	4
EXPANDR2	1	1	2.5	3
MIXER1	1	1	2.5	2
MIXER3	1	1	2.5	2
CHILLER3	2	1	3.5	2
HEATER4	[80]	0.4	2	1
DISTILL3	1+2	0.4	4	2
CYCLONE	[81]	0.3	2.5	1
DISTILL4	1+2	0.3	4	1
DISTILL2	1+2	0.2	4	1

DISTILL1	1+2	0.2	4	1
EXTRACTR	[82]	0.1	2.5	0.4
DISTILL5	1+2	0.1	4	0.4
MIXER2	1	0.1	2.5	0.2
HEATER3	2	0.1	3.5	0.2
MIXER4	1	0.05	2.5	0.1
HEATER1	2	0.04	3.5	0.1
HEATEX	1	0.0	3.5	0.1
CHILLER2	2	0.03	3.5	0.1
FLASH	2	0.0	2.5	0.1
PUMP3	1	0.02	4	0.1
HEATER2	2	0.02	3.5	0.1
CHILLER1	2	0.02	3.5	0.1
DECANTER	2	0.0	2.5	0.05
CHILLER4	2	0.02	3.5	0.1
PUMP1	1	0.01	4	0.04
PUMP2	1	0.01	4	0.03

Table B1: Capital Expense of Equipment Cost and Installed Cost

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