Production of Polyvinyl Acetate

Abrahim Yousef Imam

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Production of Polyvinyl Acetate

by

Abraham Yousef Imam

An Honors Capstone

submitted in partial fulfillment of the requirements

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of

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Honors Capstone Director: Dr. Ramon Cerro
Professor, Chemical and Materials Engineering
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Abraham Imam

Student Name (printed)

Abraham Imam

Student Signature

4/27/16

Date
Mantis

Project Feasibility Study

Date: 02-16-2016
To: Dr. Cerro, Chief Supervisor
From: Group 3

Team Lead: Jeston Thompson
Quality Assurance: Landyn Masoner
Project Engineer: Ibrahim Imam
Project Engineer: Benjamin Ballard

Executive Summary:
Mantis polymers has been requested to initiate a project feasibility study for the continuous free radical solution polymerization of vinyl acetate monomer into polyvinyl acetate (PVAc). An analysis for the practicability of this project has been performed with respect to the production aspect as well as the market assessment. For the process to produce 50,000 tons per year of PVAc, the plant will need a supply of 50,138 tons of monomer, 99 tons of initiator, and 7,520 tons of solvent per year. The raw materials will cost $49,870,085.51 per year, and the product (PVAc) will be sold for $125,000,000.00 for a gain of $75,129,914.49 profit. The current selections of solvent and initiator are methanol and 2,2 azo-bis-isobutyronitrile respectively. Methanol and 2,2 azo-bis-isobutyronitrile were selected due to their favorable kinetics and low cost. Furthermore, market analysis on the raw materials suggests a relatively stable market solidifying the team's selection. Polymerization of the monomer is designed to reach nearly 100 percent conversion with little residual monomer to eliminate the need for a recycle stream. Based on the team’s cost and economic assessment, this draft should proceed into the next phase as it is a viable option for the manufacture of PVAc.
**Identification of Problem and Needs:**

Mantis will evaluate the feasibility of a polyvinyl acetate (PVAc) manufacturing plant by implementing process engineering techniques. A minimum of 50,000 tons of PVAc must be produced annually to feed to the polyvinyl alcohol plant as a chemical intermediate. The reaction will be carried out by means of solution polymerization, and a feed inlet of solvent and vinyl acetate monomer (VAM) must enter the reactor at the proper flow rate. The process must be initiated with the thermal decomposition of the initiator entering into each of the reactors in series. The material selection is contingent upon kinetic parameters, market prices, seasonal fluctuations, and supplier fidelity and must be selected accordingly. Safety and climate analyses will also be included in the assessment.

The process must be run in either a sealed environment to prevent air impurities, or placed under a nitrogen atmosphere. The process may also involve the use of a chain transfer agent; therefore, a market analysis for chain transfer agents must also be included.

**Products and Raw Materials Specifications:**

As with most polymerizations, the molecular weight of the polymer during reaction is heavily dependent upon purity of the raw materials. It is for this reason that the selection of 99.9% and higher purity must be requested for all raw materials.

**Solvents:**

Methanol must be purchased at a purity of 99.9% or higher from a supplier. One supplier of methanol that can deliver such purity is Methanex, and they are found within 50 miles of Baton Rouge. The plant was recently built in Louisiana after the company decided to move the plant its Chile production site. The price for the pure methanol from Methanex would be approximately $0.75 per gallon, which equates to approximately $226 per ton.

Ethyl acetate must also be purchased at a purity of 99.9% or higher from the supplier. The supplier of choice for this solvent is Eastman. The plant that produces ethyl acetate is in Longview, TX, and would have to be shipped to our plant in Baton Rouge, LA. The cost of the ethyl acetate, excluding transportation costs, would be $1375 per ton.

Benzene is also being looked at as an alternative solvent. However, this would be a last option as it poses many safety and health concerns. The purity needed for benzene would be 99.9% and could be supplied by DOW Chemical located in Plaquemine, LA. The cost of the pure benzene would be $600 per ton.

<table>
<thead>
<tr>
<th>Solvent</th>
<th>Price (USD/ton)</th>
<th>Economic Price Stability</th>
<th>Distance to Plant (mi)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Methanol</td>
<td>226</td>
<td>Stable</td>
<td>26 by truck 48 by river</td>
</tr>
<tr>
<td>Ethyl Acetate</td>
<td>1370</td>
<td>Slight Fluctuations/Mostly Stable</td>
<td>300 by truck</td>
</tr>
<tr>
<td>Benzene</td>
<td>600</td>
<td>Fairly Stable</td>
<td>16 by truck 23 by river</td>
</tr>
</tbody>
</table>

Table 1: Shows the prices of the solvent options as well as their current economical stability.
Initiators:

2,2 Azo-bis-isobutyronitrile (AIBN) is the team's preferred initiator for this process. This is due to its intrinsically favorable kinetics and its low market cost and stability. AIBN will be bought from Akzo Nobel with a cost of $5,443 per ton. This is the current price; however, Akzo Nobel is planning to increase the price to $6,523 per ton in the near future. The purity of the initiator will be 99.9% and will be shipped from New Orleans, LA to our plant in Baton Rouge, LA.

Benzoyl peroxide is also an option for the use as an initiator. This raw material must be at a purity of 99.9% or higher. Benzoyl peroxide can be purchased from Shangqiu Kangmeida Biotechnology located in Henan, China. The cost of the initiator is $10,000 per ton. This initiator of course would have to be imported from China, which would add a considerable cost to shipping of the raw material.

Lauroyl peroxide was found to be utilized in small lab scale experiments with the polymerization of VAM; however, it should only be utilized during shortages due to the excessively high cost of the peroxide. The cost of this initiator is approximately $159,000 per ton from Alfa Aesar.

<table>
<thead>
<tr>
<th>Initiator</th>
<th>Price (USD/ton)</th>
<th>Distance to Plant (mi)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzoyl Peroxide</td>
<td>9,977</td>
<td>8,000</td>
</tr>
<tr>
<td>AIBN</td>
<td>5,443</td>
<td>80</td>
</tr>
<tr>
<td>Lauroyl Peroxide</td>
<td>159,000</td>
<td>1300</td>
</tr>
</tbody>
</table>

Table 2: The table above shows the price differences of the initiators and their distance to the plant.

Monomer:

The vinyl acetate monomer will be purchased at 99.9% purity with an inhibitor concentration of 3-7 ppm. The inhibitor is hydroquinone, and the initiator must overcome this concentration to begin polymerization. DOW Chemical will be the principal supplier with a cost of approximately $950 per ton. If DOW Chemical has a raw material disruption, Celanese, Dupont, and Wacker are also potential suppliers of VAM located within the vicinity of operations.

Other Raw Materials:

Depending on the reaction pathway data, nitrogen may be utilized to displace oxygen and drive the process with less impurities. Nitrogen can be purchased from Airgas at a price of $3000/m³. The plant is located 9 miles from our plant in Baton Rouge, LA.

If the team finds that a chain transfer agent is needed to control molecular weight, acetaldehyde will be purchased from Eastman at a cost of $910 per ton. The plant is located in Longview, TX and will need to be sent via tank car to our plant in Baton Rouge, LA. For smaller
quantities, Eastman has a returnable container program which may benefit our plant depending on chain transfer agent requirements.

**Product:**

The product that Mantis is making is polyvinyl acetate (PVAc). The main use of PVAc is for the production of PVA or polyvinyl alcohol. This main use requires that Mantis produces an almost pure PVAc product of 99.9%. This is due to the needed purity for the hydrolysis of PVAc to PVA. We will be selling our product at current market prices of $2,500 - $3,500 per ton based on CF Adhesive. Both low and high ends of product cost will be used in comparison since there is such a large deviation in price.

**Supply Chain Management (Light):**

![Supply Chain Diagram](image)

Figure 1: This figure shows the supply chain affiliated with Mantis.

**Solvents:**

Methanol is our company’s preferred solvent choice and will be supplied by the Methanex facility located in Geismar, LA. This particular facility was recently reassembled and has become operational as of early 2016, so a supply contract with them would allow for cheapest cost of delivery. On average, the Methanex company as a whole sold more than 8.5 million tonnes of product in 2014, which awarded them the title of world’s largest producer/supplier of methanol. In addition, methanol has become important in the search for alternate fuel sources, so the marketing of methanol is expected to increase as the economy expands. Methanol is currently sold by Methanex for $0.75/gallon or $226/ton, thus its affordability is duly noted.
Ethyl Acetate is the second solvent option our company is considering in our polymerization reaction. The supplier of it would be Eastman Chemical Company located in Longview, Texas. Eastman is a very well known chemical producing company and would be a reliable source of Ethyl Acetate if the decision was made to use it as the solvent. The market for Ethyl Acetate has been very consistent the last two years and fairly stable the last ten years as shown in Figure 2. Ethyl acetate, however, is a slightly more expensive chemical compared to methanol; the current market price of ethyl acetate is $1,367/ton.

Figure 2: This figure shows the economic trends of methanol over the last ten years in $/ton sold. [12]

Figure 3: This figure shows the economic trends of ethyl acetate over the last ten years in $/ton sold. [10]
Benzene, our final solvent consideration for our reaction, is a very corrosive chemical, but if utilized in our process the market is fairly stable as seen in Figure 3 as of the last few years. However, the major drop in 2008-2009 was due to the stock market crash, and most other fluctuations are due to crude oil prices. In addition, the supplying company would be DOW Chemical who is located 16 miles away from Baton Rouge, which would allow for a very cheap cost of transportation compared to other options.

![Benzene Prices: 10 Year Span](image)

Figure 4: This figure shows the economic trends of Benzene over the last ten years in $/ton sold. [11]

**Initiator:**

AIBN (2,2 Azobisisobutyronitrile) is the primary initiator Mantis is considering due to its high popularity use in free radical polymerization. This is mainly due to the fact that it is safer and far less explosive compared to Benzoyl Peroxide, which is a highly explosive initiator. AIBN can be considered a more effective initiator because it requires significantly less moles to instigate the reaction, thus it facilitates a more controlled process with respect to reaction rates. The suppliers market for AIBN is very limited for industrial use; therefore, the few suppliers can drive up the cost as desired. AIBN has a price of $5,443/ton coming from Akzo Nobel, located eighty miles away in New Orleans, LA. As a result, AIBN is the preferred initiator for this process.

**Monomer:**

VAM (Vinyl Acetate Monomer) is a widely used polymer component utilized in adhesives, food, plastics, textiles and many other processes. VAM’s market shows to be very stable with the exception of the 2008 stock market crash as well as the 2011 oil shock. Currently, there is a constant demand for products requiring VAM to be further polymerized so that it can be used to make commercial products. The primary effector of VAM’s market price is the stock market trends, evidenced by similar rise and fall tendencies and future speculation.

Companies such as DOW Chemical, Celanese, DuPont, and Wacker all compete in the Vinyl Acetate/Polyvinyl Acetate market, driving down the bulk cost of VAM to be $950/ton. The major deciding factor for the VAM supplier was the cost of transportation, based on the distance to our facility. Our top two choices are DOW Chemical, located 16 miles from Baton Rouge, and DuPont, located 30 miles from Baton Rouge.
Figure 5: This figure shows the top VAM producing companies worldwide. [20]

Figure 6: This figure shows the economic trends of vinyl acetate over the last ten years in $/ton sold. [13]
Other Raw Materials:

Acetaldehyde will be the chain transfer agent if it is decided that it is needed in the polymerization reaction. It is sold by Eastman Chemical Company located in Longview, Texas, for $910/ton. The market for Acetaldehyde is currently very stable and is anticipated to increase as Asian companies continue to grow, forcing a higher demand for chemical compounds.

Crude oil is a very important marketing influence that affects nearly every aspect of production. This energy source is currently being sold very cheaply at a rate of $29.50/barrel. This allows for cheaper transportation costs which can in turn reduce the manufacturing costs and hence overall cost of production. This low cost of crude oil can increase the economic standpoint of exploration of new manufacturing techniques and products, elevating demand for chemical products such as VAM and PVAc.

![WTI Crude Oil Price](image)

Figure 7: This figure shows the economic trends of crude oil over the last ten years in $/barrel sold. [21]

Polymer:

Poly Vinyl Acetate is the end product of our company, but it is our intention to sell it to our sister company. Mantis can also sell in the open market to companies like DOW and Celanese, who further process PVAc to produce PVA, adhesives, and paint. The current market value of PVAc is between $2,500 and $3,500 per ton. This variance is mainly due to economic slowdown in Europe and developing countries. However, the U.S. PVAc market is anticipated to grow at an average rate of 3% annually, so this will be beneficial to our company’s future.
Further Processing Products:

PVA (Polyvinyl Alcohol) is a water soluble synthetic polymer which can be produced from our company’s PVAc. It has many of the same uses as PVAc such as papermaking, textiles, adhesives, and a variety of coating and film uses. Some uses specific to PVA is it’s ability to package goods such as dyes, laundry, agrochemicals, and electrical applications for optical films. With all these uses, the global market of PVA is anticipated to grow 5% annually. This growth will provide our company with a high demand of PVAc from companies such as our sister company, Celanese, and DOW Chemical who make PVA, where they will then sell their polymer to companies like SyntheMed, Inc, GlassMaster Company, Oxymar, Owens Corning, Bairnco Corporation who make a variety of specialized products.

Customers Market Assessment:

Polyvinyl acetate (PVAc) is a critical constituent of adhesives and paints; thus, they are the leading markets for PVAc. The global market value for industrial grade is expected to increase by a Compound Annual Growth Rate (CAGR) of 5.13%, and it should reach a value of $10.56 billion by the year 2020. According to Figure 8, market revenues from PVAc in industrial adhesives will continue to rise gradually and at an increasing revenue range. Major contributors to the adhesives market include 3M, Henkel A&G, Bostik, and The DOW Chemical Company. Similar to other industries, the demand for construction grade adhesives is on an upward rebound following the market crash. Hence, these customers will require a constant supplier, Mantis, to continue forming their products.

Aside from the adhesives market, PVAc has some unique and innovative uses in other growing markets. Mantis is expected to supply much of its PVAc to its sister company in order to produce Polyvinyl alcohol, PVA. PVA is being incorporated into emerging biotechnologies and medical therapeutics, such as a bioresorbable polymer technology. This bioresorbable adhesion barrier film can prevent and minimize tissue scarring induced by postoperative, surgical procedures. PVA is also utilized in the production of glass wool fibers. This can be formed into specialty thermal and acoustic insulation, roofing shingles, vinyl siding, and several other coated construction materials. This has extended to the military sector for electronic coatings.

PVAc is highly versatile in its applications. A decline in a single market will not dilapidate the PVAc market, since the buyers are not directly contingent on one another. However, the ever-increasing adhesives market constitutes a larger portion of the PVAc consumers. The biomaterials market is rapidly increasing with the need for more advanced healthcare technologies; the global implantable biomaterials market has been speculated to increase at a compound annual growth rate of 6.73% and reach $133 billion by the year 2022. This market could boost the demand for PVA and PVAc, providing a second leading branch for potential consumers.
Suppliers Inventory and Trends:

Solvent:

Methanex sells Methanol at $226/ton which has remained fairly constant over the past few years. The local market climate for methanol has been generally well as of October 2015. The market price for methanol in the US has had a slight $1.50/gal increase from the month prior. Recently the range of non-discounted contract price for methanol on average is $1.55/gal - $1.80/gal.

The global market climate is also fairing well with overall demand in China increasing. Global demand for methanol in the last 5 years has grown by more than 45% to $32 billion in annual sales. Current and forecast Global demand for methanol is expected to grow another 70% over the next 6 to 7 years. Lately the methanol-to-olefin market has been a large driving force. A driving force that many say should stay fairly stable in the coming years as new ventures arise. Methanex’s production in Europe is expected to increase with the reinstatement of the manufacturing plant in Damietta, Egypt. The supply of methanol should increase because due to the fact that local methanol producing companies Celanese and Mitsui are set to start-up their joint venture 1.4m tonne/year Clear Lake facility in Texas in October and Methanex starting up another 1m tonne/year plant that it relocated to Geismar, Louisiana, by the end of 2015. These are just a few of the factors that might affect the production of methanol.

Methanol’s market trend seems to closely trail the national economic trends. If the economy hits a recession, so does methanol. However, the currently it is highly stable and has a rebound trend from previous declines. Also, as previously stated in the supply chain management, Methanex recently opened a plant in Geismar, LA which will add jobs and allow for supply of the growing need of methanol. As the economy grows, so does the need for alternative fuel sources and cleaner energy production. That demand alone should secure Methanex as a great supplier of methanol for many years to come.
Initiator:

AIBN is sold by Akzo Nobel at $5,443 per ton under the brand name Perkadox AIBN. With respect to the local market climate, much of the local market trends for the Perkadox AIBN initiator are proprietary information. However, Akzo Nobel Polymer Chemicals has announced that it will increase the price of the Perkadox AIBN product by $0.54 per pound. This would increase the expected cost of the raw material from $5,443 USD/Ton to $6,523 USD/Ton. Perkadox AIBN is also utilized by other chemical \ that specialize in the production of making synthetic rubber (specifically Styrene, Butadiene, and silicone rubber). These companies use Perkadox AIBN as a chemical blowing agents in the curing process of elastomeric compounds. East Copolymer is a potential competitor, because the company has an SBR producing plant based in Baton Rouge which produces SBR products Carbomix® and Copo®SBR.

Global market factors that affect the price of Perkadox AIBN on a global scale include both production costs and transportation costs. In 2011, an Arkema study observed how the rising costs of fuel which translates into transportation costs was responsible for driving a price increase of AIBN of € 400 per ton in Europe and $600 per ton in North America.

Factors that might affect production include the recent decline of petroleum and crude oil prices can have an effect on the transportation costs of raw products of AIBN production and should be considered when contracting a supplier for the AIBN product.

Monomer:

Vinyl acetate monomer is the primary raw material needed in Mantis’ process. The monomer will be bought at 99.9% purity from DOW Chemical as described previously.

Almost all of the production of VAM is converted for the production of PVA which is a widely utilized polymer. They are often further reacted to produce block and copolymers such as ethylene-vinyl alcohol. The vinyl acetate market is primarily an oligopoly. This is due to high costs and relative stalemate in technological advancement. As for the production of VAM, a steady shift to the Asian continents such as China and the middle east can be observed. Slowly, the Central American plants are closing down for the more favorable Chinese operations. Western Europe has also become a significant importer due to this shift, and this trend will continue, as two plants ceased operations in late 2013. As a whole, the steady shift of monomer production to China causes some slight concern as to monopolization of the production of VAM. However, with the United States and Western Europe accounting for over 50% of PVAc consumption, there is plenty of room to grow in the sector. Between 2013-2018 the U.S. alone is expected to grow in VAM consumption by 3 % per year. Global VAM demand is led by China (36%) followed by Western Europe (17%) and the United States (16%). The United States is the largest exporter of VAM in the world.
Polymer:

The product (polyvinyl acetate) will be sent down the line two another part of the plant for the final product of poly vinyl alcohol. However, the PVAc can be sold as an intermediate to companies that produce different latex compounds, paints, adhesives, PVA, and etc. Sekisui in particular could have use for our product in their polymerization step to produce their supply of PVA (Celvol®). Sekisui is important to mention because they have a plant located in Dallas, TX and specifically import polyvinyl acetate to produce PVA. Other possible buyers include Wacker Chemicals, DOW Chemicals, SyntheMed, Inc., GlassMaster Co, Oxymar, Owens Corning, Bairnco.

The Local Market Climate is expected 3% rise in the annual consumption which is predicted from 2013-2018 in the United States. This is according to a study conducted by IHS, Inc. A variety of packaging centers, chemical plants or construction companies could be included in our list of potential customers. An independent study shown by Figure 10 below shows how China accounted for over 35% of PVAc consumption in 2013. The Chinese import will be a major competitor, as our product should cater to the needs of our sister company and other local buyers. The PVAc copolymers produced in China are largely VAE and vinyl acetate/acrylic ester copolymers. PVAc is utilized for adhesives, coatings, construction and other uses worldwide and the global consumption for PVAc as an intermediate is expected to increase at more than 5% per year through 2018.
Factors that may affect production of our product may include tropical weather during certain months due to location in the Gulf Coast Area, the rise and fall of fuel costs, and the level of local competition. PVAc can be supplied as an intermediate only to a limited number of chemical plants, because it is more economical to have the raw materials to produce PVAc and break it down into finished goods on site, rather than purchasing the intermediates. Also, PVAc copolymers (containing 85% VAM and 15% n-butyl acrylate, in particular) has lost market share to higher performing all acrylic emulsions utilized in the polymer coating market.

![World Consumption of Polyvinyl Acetate—2013](image)

Figure 10: Shows the percent consumption of PVAc for the world in 2013. [17]

Other Raw Materials:

Nitrogen will be supplied by a local AirGas branch located in Baton Rouge, LA. Nitrogen is utilized in many other faculties including medical facilities, agricultural applications, and ammonium production. According to Western Plant Health Association, the US consumption of nitrogen for fertilizer production has been forecasted to be around 13 million short tons annually. There is an increasing trend for nitrogen consumption, and China is the world’s leading consumer with 30% of total global consumption. Factors that would affect our ability to obtain nitrogen for our process would include any inclement weather during tropical seasons.

Risk Management of Supply Chain:

The risk of the supply chain that we have established is relatively low due to the general stability in the local and global sectors of each product. However, the team has ensured redundancies within the supply chain so that interruptions in production are minimized. There is almost a zero risk of the loss of our Methanex supplier do to the shear size of the company. Methanex is the world's
The polymerization of vinyl acetate presents a particular kind of issue regarding the reaction mechanisms. Free radical polymerization allows for achieving a relatively quick high molecular weight. After analysis and research, the use of an individual solvent was selected versus a mixture of solvent. This is due to mixtures generally decreasing rate of polymerization in the reaction. The team is performing a chain growth addition polymerization, therefore, if needed the same equipment can be used for free radical as is used in emulsion. This will be beneficial to us as we will have a template to base our design on. Based on the safety of the reaction and conditions we have selected reactors to not exceed 10,000 gal. This will mitigate some of the risk involved in free radical polymerizations. Reactor temperatures should not drop below 62°C and should never exceed 82 °C. This is also to prevent a runaway reaction.

Before kinetic calculations can begin, a few assumptions must be made. The first assumption is that termination occurs exclusively by disproportionation. This assumption is supported by many articles on polymerization. The second assumption is that polymerization follows classical free radical polymerization. This is for the use of the differential equation that models the thermal decomposition of the initiator. The third assumption is that the monomer concentration decreases steadily
throughout the reaction and approaches zero at the end. This is a pretty self explanatory assumption, but one that must be made nonetheless. Furthermore, the team is still deciding where extraneous monomer should go. The amount is roughly 138 tons/year. The kinetics to add a feed loop to cycle polymerization is extremely complex. Small monomer amounts are being considered for the flare. The unused monomer will definitely not be stored though. This would pose a huge safety risk for explosions. These calculations are primary calculations that do not include chain transfer constants. Those constants are expected to be added to the calculations for the second report.

![Reaction Mechanism Diagram](image)

**Figure 11:** This figure illustrates the reaction mechanism for Mantis' free radical polymerization.

**Input and Outputs:**

- **Initiator-** 99 tons/year
- **Polymer-** 50,000 tons/year
- **Monomer-** 50,138 tons/year
- **Solvent-** 7,520 tons/year
- **Possible Nitrogen Input**
- **Option for residual monomer-** 138 tons/year

**Figure 12:** This figure illustrates the input and output amounts of the reaction
As shown above, the initiator enters the process at approximately 99 tons/year. The monomer enters at 50,138 tons/year along with the solvent at 7520 tons/year. The reaction conditions are 65°C with a possible slight pressure to prevent volatile boiling of methanol. This would be accomplished with the nitrogen produced during the decomposition of the initiator. If more nitrogen is needed for pressurization, it can be purchased readily. These conditions lead to a 99.724% conversion of monomer. Options for the residual monomer are still being discussed.

**Gross Material Balance and Economic Analysis:**

<table>
<thead>
<tr>
<th>Initiator (tons/yr)</th>
<th>Monomer (tons/yr)</th>
<th>Solvent (tons/yr)</th>
<th>Polymer</th>
<th>Profit/year</th>
</tr>
</thead>
<tbody>
<tr>
<td>AIBN</td>
<td>99.0137</td>
<td>VAm</td>
<td>50,138.38</td>
<td>Methanol</td>
</tr>
</tbody>
</table>

Table 4: This table illustrates Mantis' decision making process when determining the appropriate materials for polymerization. This information was then used to produce table 5.

<table>
<thead>
<tr>
<th>Initiator</th>
<th>Monomer</th>
<th>Solvent</th>
<th>Polymer</th>
<th>Profit/year</th>
</tr>
</thead>
<tbody>
<tr>
<td>Benzoyl Peroxide</td>
<td>$989,703.00</td>
<td>$47,631,462.84</td>
<td>Benzene</td>
<td>$4,512,000</td>
</tr>
<tr>
<td>AIBN</td>
<td>$538,931.52</td>
<td>$47,631,462.84</td>
<td>Methanol</td>
<td>$1,699,691.15</td>
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<tr>
<td>Lauryl Peroxide</td>
<td>$15,741,000</td>
<td>$47,631,462.84</td>
<td>Methanol</td>
<td>$1,699,691.15</td>
</tr>
</tbody>
</table>

Table 5: This table illustrates Mantis' decision making process when determining the appropriate materials for polymerization. Green is the preferred method, orange is less optimum, and red is not recommended. All values were based on one set of materials balance.


**References:**

**Price:**

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Kinetics:

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[31] Corrosion with methanol

http://chromsci.oxfordjournals.org/content/23/1/22.abstract

[32] Corrosion with methanol

http://emsh-ngtech.com/methanol/our-methanol/

**Consumers/Suppliers:**

[33] Methanol Info:

http://www.usmeoh.com/

[34] Methanol Raw Material/ Source:


[35] Vinyl Acetate Top Producers chart:


**PVA Buyers:**

[36] SyntheMed, Inc.:


[37] Owens Corning:


[38] Bairnco Corp:


**Misc:**

Mantis
Project Feasibility Study

Date: 04-05-2016
To: Dr. Cerro, Chief Supervisor
From: Group 3 - Phase II

Team Lead: Ibrahim Imam
Quality Assurance: Benjamin Ballard
Project Engineer: Landyn Masoner
Project Engineer: Jeston Thompson

**Executive Summary:**

The design of Mantis’ continuous free radical solution polymerization process entails a stir reactor, recycle stream, and stripping column to produce polyvinyl acetate. The reactor will be jacketed to prevent a thermal runaway and to accurately control the reaction. AIBN, methanol, and vinyl acetate monomer will enter the reactor at 76.50 kg/hr, 5669.382 kg/hr, and 1000.479 kg/hr respectively. The design process will reach 97.6% conversion after 4 hours and exit the reactor. Next, 7 ppm of hydroquinone in 500 kg/hr methanol will be added to the polymer solution to terminate polymerization at the desired molecular weight. Stream S32 is then stripped, separating 137.77 kg/hr vinyl acetate vapors from the polymer. The unreacted monomer is then cooled to 23°C to be recycled into mixer M1 prior to entering heat exchanger HEX 1. During the reaction, the thermal degradation of the initiator will produce one mole of Nitrogen for every mole of initiator that is degraded. This will allow polymerization in an oxygen free environment. The final stream S33 will contain the polymer in solution with methanol with a planned purity of 99% at 5531.616 kg/hr, which converts to 50,000 tons/year of polyvinyl acetate.
Figure 1: This flow sheet contains all valve names and unit op names.
Figure 2: This flow sheet contains all stream names.
Flowsheet Parameters for Sizing of Major equipment:

<table>
<thead>
<tr>
<th>Flowsheet ID</th>
<th>Unit Ops</th>
<th>Area (m²)</th>
<th>Diameter (m)</th>
<th>Height/Length (m)</th>
<th>Volume (m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>Reactor</td>
<td></td>
<td>2.8</td>
<td>6</td>
<td>37</td>
</tr>
<tr>
<td>HEX 1</td>
<td>Heat exchanger</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HEX 2</td>
<td>Heat exchanger</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>HEX 3</td>
<td>Heat exchanger</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C1</td>
<td>Condenser</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C2</td>
<td>Condenser</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DT1</td>
<td>Day Tank</td>
<td>59.79</td>
<td>2.6</td>
<td>6</td>
<td>32</td>
</tr>
</tbody>
</table>

Table 1: This table represents the values used in sizing equipment for pricing and purchase. (This table is tentative table.)

Separation Sequences:

This process will entail a feedback loop to recycle the unreacted vinyl acetate. A stripping column (PSC) is used to remove unpolymerized vinyl acetate from the polyvinyl acetate solution leaving reactor (R3). Methanol vapors will be used to strip vinyl acetate from the solution. The overhead fraction from the stripping column consisting of solvent, vinyl acetate and any nitrogen gas produced by the reaction will be directly recycled and fed back into the reactor. The stream will leave the stripping column and directly enter a heat exchanger HEX 2 to cool the stream down to 23°C. Cooling the stream from HEX 2 along with adding hydroquinone to terminate the polymerization are examples of built-in safety parameters. A recycle stream was added to reduce costs and to prevent the separation of an azeotrope that forms with the methanol and vinyl acetate. The vinyl acetate content in the bottom effluent from the stripping column is reduced to less than 0.07 wt%. This is optimal due to higher concentrations leading to an acetaldehyde formation and subsequent yellowing of the solution. The team is still designing the stripping column as the bottom of the striper is expected to be highly viscous (between 1-50 Pa*s). For the reactor size, the team decided on a one hour safety volume extra to prevent damage to the reactor. With flow rate only the consideration, and taking into account a residence time of 4 hours, the
reactor volume was calculated to be 29.611 m$^3$. With the addition of the one hour cushion, it brings the volume to approximately 37 m$^3$. This in turn led to design specifications of a 6 meter height by 2.8 meter internal diameter. The team is still compiling the table and computing data for the separation sequences.

<table>
<thead>
<tr>
<th>Flowsheet ID</th>
<th>Unit Op</th>
<th>Duty</th>
<th>Temp (In/out)</th>
<th>Pressure (In/out)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>Reactor</td>
<td></td>
<td>65°C/65°C</td>
<td>16 psia/16 psia</td>
</tr>
<tr>
<td>HEX 1</td>
<td>Heat exchanger</td>
<td>159.44 kW</td>
<td>23°C/65°C</td>
<td>16 psia/16 psia</td>
</tr>
<tr>
<td>HEX 2</td>
<td>Heat exchanger</td>
<td>116.65W</td>
<td>65°C/23°C</td>
<td>16 psia/16 psia</td>
</tr>
<tr>
<td>HEX 3</td>
<td>Heat exchanger</td>
<td>185.15W</td>
<td>23°C/70°C</td>
<td>16 psia/16 psia</td>
</tr>
<tr>
<td>C1</td>
<td>Condenser</td>
<td></td>
<td>67°C/65°C</td>
<td>16 psia/16 psia</td>
</tr>
<tr>
<td>C2</td>
<td>Condenser</td>
<td></td>
<td>70°C/65°C</td>
<td>16 psia/16 psia</td>
</tr>
<tr>
<td>M1</td>
<td>Mixer</td>
<td>N/A</td>
<td>23°C/23°C</td>
<td>16 psia/16 psia</td>
</tr>
<tr>
<td>M2</td>
<td>Mixer</td>
<td>N/A</td>
<td>65°C/65°C</td>
<td>16 psia/16 psia</td>
</tr>
<tr>
<td>M3</td>
<td>Mixer</td>
<td>N/A</td>
<td>65°C/65°C</td>
<td>16 psia/16 psia</td>
</tr>
<tr>
<td>PSC</td>
<td>Polymer Stripping Column</td>
<td></td>
<td>65°C/65°C</td>
<td>16 psia/16 psia</td>
</tr>
<tr>
<td>LVS</td>
<td>Liquid/Vapor Separator</td>
<td></td>
<td>65°C/70°C</td>
<td>16 psia/16 psia</td>
</tr>
</tbody>
</table>

Table 2: This table represents the different parameters for each of the given streams. (This table is tentative.)
Heat Recovery System:

For the system above, the design will require the following: two heat exchangers, one condenser on the reactor, R1, and a condenser after the stripping section to cool the recycle stream down to 23°C. Considering safety precautions, further research is required to determine the placement of a heat recovery network. To note, vinyl acetate is a very unstable reactant which means that additional safety precautions and redundancies are needed to be in place to prevent explosions. It will be decided to incorporate redundancies while maximizing heat recovery with the heat exchangers HEX 1, HEX 2, and the condensers C1, and C2.

Considering the cooling system for the reactor, it has been determined that using a cooling-jacket design will be the most optimum choice for maintaining the temperature of the reactor. This type of cooling is the most commonly preferred method to all other types of cooling when conducting a free radical polymerization. In addition to the cooling jacket, methanol vapor from the reactor will be recycled to assist in regulating the temperature of the reaction mixture and cutting chemical costs. This will be accomplished by the use of condenser C1.

Material and Energy Balances:

For phase two, the team was requested to use Chemcad to produce stream data, material balances, and energy balances. However, the polymer module for Chemcad requires the additional dynamic module. Furthermore, the polymer module does not contain the necessary components for our polymerization reaction. The team has opted to produce a flow sheet and operations from Chemcad; however, the calculations for the material and energy balances will be done with the use of excel and Mathcad.

During free radical polymerizations, the AIBN decomposes into two radicals and elemental Nitrogen. The AIBN will then react to form a monomer radical to begin polymerization. The mechanism causes many different lengths of monomers leading to a PDI or poly dispersity index, where, a majority of the chain lengths are the desired chain length and some residual chains are undesired smaller chain lengths. Nonetheless, the AIBN is one hundred percent consumed by the monomer or converted to Nitrogen.
Please see Appendix B for sample calculations for the mass balances of the system. Computing the heat balances and finalizing the mass balances will be a working progress. The next step will be to confirm all hand calculations for precision following the cost estimation of the major components of the process design.

**Safety Analysis (HAZOP):**

<table>
<thead>
<tr>
<th>Study Node</th>
<th>Name</th>
<th>Purpose</th>
</tr>
</thead>
<tbody>
<tr>
<td>C 1 – C 2</td>
<td>Condenser</td>
<td>Condenses vapors into liquid for recycle</td>
</tr>
<tr>
<td>DT 1</td>
<td>Storage Day Tank</td>
<td>Stores solvent-initiator mixture and VAM</td>
</tr>
<tr>
<td>H 1</td>
<td>Hopper</td>
<td>Allows methanol and AIBN to flow into ST 1</td>
</tr>
<tr>
<td>HEX 1 – HEX 3</td>
<td>Heat Exchanger</td>
<td>Transfers heat to and from mixture</td>
</tr>
<tr>
<td>LVS</td>
<td>Liquid-Vapor Separator</td>
<td>Separates vapors from recycle monomer</td>
</tr>
<tr>
<td>M 1 – M 3</td>
<td>Mixer</td>
<td>Mixes AIBN into polymer reactors</td>
</tr>
<tr>
<td>P 1 – P 9</td>
<td>Pump</td>
<td>Increases pressure and flow</td>
</tr>
<tr>
<td>PSC</td>
<td>Polymer Stripping Column</td>
<td>Removes impurities from polymer product</td>
</tr>
<tr>
<td>R 1</td>
<td>Reactor</td>
<td>Performs polymerization reaction</td>
</tr>
</tbody>
</table>

Table 3: HAZOP study node identification

<table>
<thead>
<tr>
<th>Study Node</th>
<th>Item</th>
<th>Parameters</th>
<th>Deviations</th>
<th>Causes</th>
<th>Consequences</th>
<th>Actions</th>
</tr>
</thead>
<tbody>
<tr>
<td>C 1 – C 2</td>
<td>2A</td>
<td>Toxic Materials</td>
<td>None</td>
<td>Inherent</td>
<td>Health hazards</td>
<td>Assess health risks and establish safety precautions</td>
</tr>
<tr>
<td></td>
<td>2H</td>
<td>Corrosion</td>
<td>Corrosion of tubes</td>
<td>Methanol vapor</td>
<td>Equipment failure</td>
<td>Proper maintenance</td>
</tr>
<tr>
<td></td>
<td>2I</td>
<td>Flow</td>
<td>Leakage</td>
<td>Improper seal</td>
<td>Off-spec product</td>
<td>Maintain seals</td>
</tr>
<tr>
<td></td>
<td>2J</td>
<td>Temperature</td>
<td>Low</td>
<td>Heater malfunction</td>
<td>Off-spec product</td>
<td>Install controller</td>
</tr>
<tr>
<td>DT 1</td>
<td>2A</td>
<td>Toxic Materials</td>
<td>None</td>
<td>Inherent</td>
<td>Health hazards</td>
<td>Assess health risks and establish safety precautions</td>
</tr>
<tr>
<td></td>
<td>1A</td>
<td>Temperature</td>
<td>Greater</td>
<td>Runaway reaction</td>
<td>Vessel rupture</td>
<td>Evaluation of the cooling water source</td>
</tr>
<tr>
<td></td>
<td>1C</td>
<td>Flow</td>
<td>Less cooling water</td>
<td>Pipe blockage</td>
<td>Temperature of process fluid remains constant</td>
<td>High temperature alarm</td>
</tr>
<tr>
<td></td>
<td>2E</td>
<td>Pressure</td>
<td>More pressure on tube side</td>
<td>Failure of process fluid valve</td>
<td>Bursting of tube</td>
<td>Install high pressure alarm</td>
</tr>
<tr>
<td></td>
<td>2H</td>
<td>Corrosion</td>
<td>Corrosion of tube</td>
<td>Hard water</td>
<td>Less cooling and tube cracking</td>
<td>Proper maintenance</td>
</tr>
<tr>
<td>HEX 1 – 3</td>
<td>1A</td>
<td>Temperature</td>
<td>Greater</td>
<td>Runaway reaction</td>
<td>Vessel rupture</td>
<td>Evaluation of the cooling water source</td>
</tr>
<tr>
<td></td>
<td>1C</td>
<td>Flow</td>
<td>Less cooling water</td>
<td>Pipe blockage</td>
<td>Temperature of process fluid remains constant</td>
<td>High temperature alarm</td>
</tr>
<tr>
<td></td>
<td>2E</td>
<td>Pressure</td>
<td>More pressure on tube side</td>
<td>Failure of process fluid valve</td>
<td>Bursting of tube</td>
<td>Install high pressure alarm</td>
</tr>
<tr>
<td></td>
<td>2H</td>
<td>Corrosion</td>
<td>Corrosion of tube</td>
<td>Hard water</td>
<td>Less cooling and tube cracking</td>
<td>Proper maintenance</td>
</tr>
<tr>
<td>LVS</td>
<td>2A</td>
<td>Toxic Materials</td>
<td>None</td>
<td>Inherent</td>
<td>Health hazards</td>
<td>Assess health risks and establish safety precautions</td>
</tr>
<tr>
<td></td>
<td>2E</td>
<td>Level</td>
<td>High</td>
<td>Low flow</td>
<td>Condensed liquid backflow</td>
<td>Install high level alarm</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Low</td>
<td>Leakage</td>
<td>Level decrease</td>
<td>Schedule inspection</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2H</td>
<td>Corrosion</td>
<td>Corrosion of column</td>
<td>Methanol vapor</td>
<td>Equipment failure</td>
<td>Proper maintenance</td>
</tr>
<tr>
<td></td>
<td>2I</td>
<td>Flow</td>
<td>Less</td>
<td>Improper seal</td>
<td>Off-spec product</td>
<td>Maintain seals</td>
</tr>
<tr>
<td></td>
<td>2J</td>
<td>Temperature</td>
<td>High</td>
<td>Heater malfunction</td>
<td>Off-spec product</td>
<td>Install temp sensor</td>
</tr>
</tbody>
</table>
Table 4: HAZOP nodal analysis

To understand and produce an effective safety protocol, the dangers of the plant must be defined. The major dangers of polymerization of vinyl acetate are its high flammability, ability of its vapor to cause flash fire, spontaneous polymerization by cross-contamination, inhibitor depletion, and exposure to heat, radiation, oxidizing materials or strong acids or bases. This in turn may result in heat generation, rapid vaporization of VAM, and possible vessel explosion. VAM is a reactive molecule. Unless inhibited, or if proper handling and storage precautions are not met, VAM can polymerize uncontrollably. VAM is typically transported in a polymerization inhibiting solution, generally hydroquinone (HQ). Properly inhibited, VAM is stable under recommended storage conditions. Prolonged or intense exposure to heat, sunlight, ultraviolet light or x-rays may result in polymerization. Spontaneous polymerization may also result from exposure to amines, strong acids, alkalis, silica, alumina, oxidizing agents (e.g., peroxides, hydroperoxides, hydrogen peroxide) or polymerization initiators. Heat and pressure generated during such polymerization may rupture insufficiently vented containers, leading to liquid spill, vapor generation, and possibly fire. The following list describes a few of the safety protocols that the team felt were necessary.

1. **MSDS - Process safety management (PSM), Engineering Supervisors, and Crew Leaders** are responsible for reviewing the MSDS and training every operator or authorized personnel on the SOP prior to proceeding to any portion of the process for the following materials: Vinyl Acetate Monomer, AIBN (Initiator), Methanol, Nitrogen, and other process materials listed in the SOP.
2. **Warning signs and warning tape/labels** are to posted where and when appropriate. It is the Engineering Supervisor and Safety Coordinator's responsibility to ensure that this is done appropriately.
3. All operators/authorized personnel are required to present a safety permit prior to entering PSM areas. This will confirm that everyone in the area has been properly trained before entering the PSM area.
4. Personal Protective Equipment (PPE) shall be worn at all times, this will include Flame Resistant (FR) Clothing, hard-hat with face shield attached (depending on work environment), chemical/cut resistant gloves, ear plugs, safety glasses, rubber steel-toe boots, and chemical suit if needed. Crew leaders and shift managers are responsible for having inventory of PPE in the control room.
5. No eating, drinking, or smoking except in designated areas.
6. Fire extinguishers and eyewash stations should be inspected regularly.
7. A safe-work permit is required prior to working on any pump, valve, or performing any maintenance on process equipment.
8. Engineering supervisors, safety coordinator, and crew leaders are to conduct a safety meeting and develop a plan of action (POA) prior to any maintenance requiring confined space/vessel entry during normal operation. The Safety Coordinator must sign and approve of a confined space/vessel permit.
9. Lock-Out/Tag-Out procedures are to be reviewed by the engineering supervisor and assigned to the operators by the crew leader.
10. Once a confined space permit is signed, operators will use a sniffer tool (air-analyzer) and submit an inspection sheet to the crew leader for approval.
11. In the case of an accident, administer first aid if applicable, and seek the on-site medical facility immediately and inform the shift manager to report the incident with 24 hours.
12. For serious accident, notify the emergency medical services immediately and report the incident within 24 hours when convenient.
13. All fire/emergency evacuation procedures are required to be reviewed by every person within the area prior to entering the area.
<table>
<thead>
<tr>
<th>Organization/Agency</th>
<th>Limit</th>
</tr>
</thead>
<tbody>
<tr>
<td>NIOSH</td>
<td>15 minute Ceiling Limit of 4 ppm</td>
</tr>
<tr>
<td>ACGIH</td>
<td>8 hour Threshold Limit Value (TLV) Time-Weighted Average (TWA) of 10 ppm</td>
</tr>
<tr>
<td></td>
<td>15 minutes Short-term Exposure Limit (STEL) of 15 ppm</td>
</tr>
<tr>
<td>Canada (Alberta, British Columbia, Ontario)</td>
<td>8 hour Time-Weighted Average (TWA) of 10 ppm</td>
</tr>
<tr>
<td></td>
<td>15 minutes Short-term Exposure Limit (STEL) of 15 ppm</td>
</tr>
<tr>
<td>Mexico</td>
<td>8 hour Time-Weighted Average (TWA) of 10 ppm</td>
</tr>
<tr>
<td></td>
<td>15 minutes Short-term Exposure Limit (STEL) of 20 ppm</td>
</tr>
<tr>
<td>EU SCOEL</td>
<td>Proposed OEL of 5 ppm (17 mg/m³)</td>
</tr>
<tr>
<td>China</td>
<td>8 hour Time-Weighted Average (TWA) of 10 mg/m³</td>
</tr>
<tr>
<td></td>
<td>15 minutes Short-term Exposure Limit (STEL) of 15 mg/m³</td>
</tr>
</tbody>
</table>

Table 5: This table demonstrates the occupational exposure limits of VAM. NIOSH is the organization that has authority in the US.

**Safety Data Sheets:**

Acetaldehyde:
https://www.fishersci.com/shop/msdsproxy?productName=AC175290050&productDescription=ACETALDEHYDE-D4%252C+99%252B+ATO+5GR&catNo=AC17529-0050&vendorId=VN00032119&storeld=10652

AIBN:
http://terpconnect.umd.edu/~choi/MSDS/Sigma-Aldrich/2,2'-AZOBISOBUTYRONITRILE.pdf

Hydroquinone:

Methanol:
https://www.airgas.com/msds/001065.pdf
Vinyl Acetate:
https://www.fishersci.com/shop/msdsproxy?productName=O50574&productDescription=VINYL+ACETATE+REAG+4LITERS&catNo=O5057-4&vendorId=VN00033897&storeId=10652

Polyvinyl Acetate:
https://www.fishersci.com/shop/msdsproxy?storeId=10652&productName=AC183250010

Nitrogen:
https://www.airgas.com/msds/001040.pdf

Water:

References:

Safety Information:

Appendix A Nomenclature:

f=efficiency factor of AIBN
I_0=Initial initiator concentration
I=Initiator concentration remaining
k_c=Rate constant for the decomposition of the initiator
k_p=Rate constant of propagation
k_t=Total rate constant
k_{td}=Rate constant for termination by means of disproportionation
k_{tr}=Rate constant for chain transfer
M_0= initial Monomer
M=Monomer remaining
MW_{solv}=Molecular weight of solvent
MW_{VAM}=Molecular weight of Monomer
R_i=Rate of initiation
R_p=Rate of polymerization
R_t=Rate of termination
\rho_{solv}= Density of solvent
\rho_{VAM}=Density of Monomer
t=time
v=chain length of the polymer
X_n=number average degree of polymerization
Appendix B Sample Calculations:

Defined variables.

\[ MW_{\text{Monomer}} := 86.09 \ \text{g mol}^{-1} \quad MW_{\text{Methanol}} := 32.04 \ \text{g mol}^{-1} \quad MW_{\text{AIBN}} := 164 \ \text{g mol}^{-1} \]

\[ \rho_{\text{Vinyl Acetate}} := 934 \ \text{g L}^{-1} \quad \rho_{\text{Methanol}} := 792 \ \text{g L}^{-1} \quad Monomer_{\text{Initial}} := 13.8 \ \text{mol L}^{-1} \]

\[ Mass\_Flow_{\text{Monomer}} := 5669.382 \ \text{kg hr}^{-1} \quad Initiator_{\text{Initial}} := 0.36877 \ \text{mol L}^{-1} \]

\[ t := 4 \ \text{hr} \quad k_d := 5.01 \times 10^{-4} \ \text{s}^{-1} \quad k_t := 6.40 \times 10^8 \ \text{mol L}^{-1} s^{-1} \quad k_p := 2300 \ \text{mol L}^{-1} s^{-1} \quad f := 0.6 \ \frac{\text{mol}^2}{L^2} \]

Monomer Mass flow rate calculations.

\[ Initiator := Initiator_{\text{Initial}} \exp (-k_d \cdot t) = 0.000271 \ \frac{\text{mol}}{L} \]

\[ M_{\text{Complex}} := \left( \frac{f \cdot k_d}{k_t} \right)^{0.5} \cdot \text{Initiator}^{0.5} = (1.129 \times 10^{-8}) \ \frac{\text{mol}}{L} \]

\[ Monomer := Monomer_{\text{Initial}} \exp (-2300 \cdot 1.129 \times 10^{-8} \cdot 14400) = 9.495 \ \frac{\text{mol}}{L} \]

\[ X_n := \frac{k_p \cdot Monomer}{2 \cdot (k_t \cdot f \cdot k_d \cdot Initiator)^{0.5}} = 1511 \]

\[ Monomer_{\text{needed}} := 65854.127 \ \frac{\text{mol}}{\text{hr}} \]

\[ Mass\_Flow_{\text{Monomer}} := Monomer_{\text{needed}} \cdot (MW_{\text{Monomer}}) = 5669.382 \ \frac{\text{kg}}{\text{hr}} \]

Solvent mass flow rate based on monomer mass flow rate. The mass flow ratio of monomer to solvent is 85/15 wt% based on journal articles and polymer chemistry textbooks.

\[ Mass\_Flow_{\text{Solvent}} := Mass\_Flow_{\text{Monomer}} \cdot \left( \frac{15}{85} \right) = 1000.479 \ \frac{\text{kg}}{\text{hr}} \]
AIBN mass flow rate calculation based on monomer concentration equations.

\[ \text{Mass Flow}_{\text{Solvent}} = 1000479.14 \ \frac{gm}{hr} \]

\[ \text{Volume}_{\text{Solvent}} = \frac{\text{Mass Flow}_{\text{Solvent}}}{\rho_{\text{Methanol}}} = 1263.231 \ \frac{L}{hr} \]

\[ \text{Molar Flow}_{\text{Initiator}} = \text{Initiator}_{\text{Initial}} \cdot \text{Volume}_{\text{Solvent}} = 465.842 \ \frac{mol}{hr} \]

\[ \text{Mass Flow}_{\text{Initiator}} = \text{Molar Flow}_{\text{Initiator}} \cdot MW_{\text{AIBN}} = 76.398 \ \frac{kg}{hr} \]

**Initial Inlet Stream Values:**

\[ \text{Mass Flow}_{\text{Initiator}} = 76.398 \ \frac{kg}{hr} \]

\[ \text{Mass Flow}_{\text{Solvent}} = 1000.479 \ \frac{kg}{hr} \]

\[ \text{Mass Flow}_{\text{Monomer}} = 5669.38 \ \frac{kg}{hr} \]

**Initial Outlet Stream Values:**

\[ \text{Mass Recycle}_{\text{Monomer}} = 137.766 \ \frac{kg}{hr} \]

\[ \text{Mass Flow}_{\text{Polym er}} = 5531.62 \ \frac{kg}{hr} \]

\[ \text{Mass Flow}_{\text{SolventInit}} = \text{Mass Flow}_{\text{Solvent}} + \text{Mass Flow}_{\text{Initiator}} = 1076.877 \ \frac{kg}{hr} \]

\[ \text{Molar Flow}_{\text{Nitrogen}} = \frac{\text{Mass Flow}_{\text{Initiator}}}{MW_{\text{AIBN}}} = 465.842 \ \frac{mol}{hr} \]

\[ \text{Mass Flow}_{\text{Nitrogen}} = \text{Molar Flow}_{\text{Nitrogen}} \cdot 14.01 \ \frac{gm}{mol} = 6.526 \ \frac{kg}{hr} \]
Reactor Sizing:

\[ t_{\text{Residence}} = 4 \, \text{hr} \]

\[ \rho_{\text{AIBN}} = 1.1 \times 10^3 \frac{\text{gm}}{\text{L}} \quad \rho_{\text{Methanol}} = 792 \frac{\text{gm}}{\text{L}} \quad \rho_{\text{Vinyl Acetate}} = 934 \frac{\text{gm}}{\text{L}} \]

\[ \text{Mass Flow}_{\text{Initiator}} = 76.398 \frac{\text{kg}}{\text{hr}} \quad \text{Mass Flow}_{\text{Solvent}} = 1000.479 \frac{\text{kg}}{\text{hr}} \quad \text{Mass Flow}_{\text{Monomer}} = 5669.38 \frac{\text{kg}}{\text{hr}} \]

\[ V_{\text{Flow}} = \frac{\text{Mass Flow}_{\text{Initiator}}}{\rho_{\text{AIBN}}} + \frac{\text{Mass Flow}_{\text{Solvent}}}{\rho_{\text{Methanol}}} + \frac{\text{Mass Flow}_{\text{Monomer}}}{\rho_{\text{Vinyl Acetate}}} = 7.403 \frac{\text{m}^3}{\text{hr}} \]

\[ V_{\text{Flow}} = 1955.582 \frac{\text{gal}}{\text{hr}} \]

\[ \text{Tot}_{\text{React. Vol}} = V_{\text{Flow}} \cdot t_{\text{Residence}} = 7822.328 \text{ gal} \]

\[ \text{Tot}_{\text{React. Vol}} = 29.611 \text{ m}^3 \]

A one hour safety buffer will be added to the overall volume of the reactor in the case of a clog or unit malfunction.

\[ \text{Tot}_{\text{React. Volume Safety Buffer}} = \text{Tot}_{\text{React. Vol}} + V_{\text{Flow}} \cdot 1 \frac{\text{hr}}{} = 37.013 \text{ m}^3 \]

After the total reactor volume was found, the dimensions were decided upon as a team.

\[ \text{Tot}_{\text{React. Volume Safety Buffer}} = 37.013 \text{ m}^3 \]

\[ \text{Height} = 6 \text{ m} \quad \text{Diameter} = 2.8 \text{ m} \]

\[ \text{Area} = \left( \frac{\pi}{4} \right) \cdot (\text{Diameter})^2 = 6.158 \text{ m}^2 \]

\[ \text{Volume} = \text{Area} \cdot \text{Height} = 36.945 \text{ m}^3 \]

Therefore, the reactor specifications are 6 meters high by 2.8 meters in diameter.
Mantis
Project Feasibility Study

Date: 04-21-2016
To: Dr. Cerro, Chief Supervisor
From: Group 3 - Phase III

Team Lead: Landyn Masoner
Quality Assurance: Jeston Thompson
Project Engineer: Benjamin Ballard
Project Engineer: Ibrahim Imam

Executive Summary:

Mantis Polymers has successfully designed a cost-effective system for the production of Polyvinyl Acetate from Vinyl Acetate Monomer. The most optimal design configuration for the production plant utilizes a continuous, free-radical, solution polymerization process. The result of this system is 99.9% pure polyvinyl acetate product. Due to its high versatility in local industries, Mantis Polymers has been tasked to produce 50,000 US tons of polyvinyl acetate per year, thereby satisfying the demands of the consumer. In order to fulfill this demand, a total amount of 50,323 tons per year of vinyl acetate monomer, 21,567 tons per year of methanol, 1,649 tons per year of AIBN, and half a ton of hydroquinone per year will be necessary. After a stringent market and economic analysis, it has been discerned that the investment will be profitable. The yearly net profit of $8,284,000.00 with an $19,354,000.00 initial investment will yield a 43% return on investment. This will in turn lead to a payback period of approximately 8 months. After careful consideration, Mantis polymers believes the process to have a medium to high risk (25%). Mantis Polymers has validated the efficacy of constructing this facility and approves this project.
Polymerization Flowsheet:

Reaction Kinetics and Flow Diagram Analysis:

To initialize the process, F1 will be introduced to A1 by means of a Hopper (H1). The F1 reactant will be mixed with the F2 stream of methanol to produce a mixture. These will in turn be pumped by P1 from A1 in stream S1 to M1. F3, containing the vinyl acetate monomer, will be pumped by P2 to M1 where the recycle stream (S15), S1, and F3 will combine. The resulting stream S2 will enter HX1 where it will be heated to the reaction temperature of 65 degrees C. After leaving HX1 the reactants will mix with the condensate (S6) in M2 and enter R1. The reactor R1 will commence polymerization once the temperature of the reactor reaches 65
degrees C. This reaction will be held at a pressure of approximately 133,000 Pa. This pressure is optimal to prevent any oxygen from entering the system. Furthermore, the reaction temperature will produce 79.152 kg/hr of vinyl acetate and methanol vapors with 13.048 kg/hr of Nitrogen. The pressure of R1 will be regulated with a pressure control system that purges Nitrogen from C1 produced. Also, there will be a rupture disk installed on R1 in the event that the pressure control system fails. The rupture disk will be rated at 405,300 Pa and will prevent the destruction of the reactor due to an explosion. The temperature scheme can be shown by Figure 1, which illustrates the temperature coming to steady state at 65 degrees C after approximately 10 minutes. The temperature of the cooling water on R1 will enter 23 degrees C and exits at 337.75 degrees C.

![Graph](image)

**Figure 1:** This graph demonstrates the reaction temperature reaching steady state after approximately 10 minutes.

The reactor (R1) will have a residence time of 4 hours allowing the polymer to reach 130,000 molecular weight or \( X_n = 1500 \) units. After the polymer leaves R1, hydroquinone will enter M3 through F4 at 7 ppm to halt the reaction and preserve molecular weight. The polymer solution will then enter a devolatilization system (DU) where the polymer, residual monomer, isobutyronitrile, and unused hydroquinone will be stripped. The polymer will then exit the system through S10 at a purity of 99.9% in a solution of methanol. The separated vinyl acetate monomer solution will leave the (DU) in S9 and enter the (DC) to separate the residual monomer and methanol from the hydroquinone and isobutyronitrile. The bottoms waste (isobutyronitrile and hydroquinone) will exit through S12 to be disposed of by waste management. The distillate stream (S15) will exit the DC at 71 degrees C and pass through
pump P5. At this point, the monomer solution will be cooled down to 23 degrees C by the use of HX3. This is a safety precaution to limit the explosive capabilities of the vinyl acetate monomer. The S15 will then be recycled back to M1 where it will combine with S1 and F3.

In an attempt to save money, Mantis explored the feasibility of introducing a heat exchanger network to cool the recycle stream. The desire was to use the exit stream of the heating utility from S3, which exits HX1 at 47.9 degrees C, to help cool down S15 from 71 degrees C to 23 degrees C. However, after pricing the size of the new heat exchangers that would be required in this network, it was decided that using a heat exchanger network would be infeasible due to an extensive return on investment.

<table>
<thead>
<tr>
<th>Flowsheet ID</th>
<th>Unit Ops</th>
<th>Area (m²)</th>
<th>Diameter (m)</th>
<th>Height/Length (m)</th>
<th>Volume (m³)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>Reactor</td>
<td>N/A</td>
<td>2.929</td>
<td>5.998</td>
<td>40.5</td>
</tr>
<tr>
<td>HX 1</td>
<td>Heat exchanger</td>
<td>25.56</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>HX 2</td>
<td>Heat exchanger</td>
<td>32.45</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>HX 3</td>
<td>Heat exchanger</td>
<td>7.75</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>C1</td>
<td>Condenser</td>
<td>1.39</td>
<td>N/A</td>
<td>N/A</td>
<td>N/A</td>
</tr>
<tr>
<td>A1</td>
<td>Agitator Tank</td>
<td>N/A</td>
<td>1.26</td>
<td>2</td>
<td>2.49</td>
</tr>
<tr>
<td>DU</td>
<td>Devolatilization Unit</td>
<td>N/A</td>
<td>2.41</td>
<td>4</td>
<td>18.23</td>
</tr>
<tr>
<td>DC</td>
<td>Distillation Column</td>
<td>N/A</td>
<td>2.44</td>
<td>15.24</td>
<td>71.17</td>
</tr>
</tbody>
</table>

Table 1: This table highlights the properties for the given unit ops on the flowsheet.
<table>
<thead>
<tr>
<th>Flowsheet ID</th>
<th>Unit Op</th>
<th>Duty</th>
<th>Temp (In/out)</th>
<th>Pressure (In/out)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>Reactor</td>
<td>81709 kW</td>
<td>65°C/65°C</td>
<td>133 kPa/ 133 kPa</td>
</tr>
<tr>
<td>HX 1</td>
<td>Heat exchanger</td>
<td>195.73 kW</td>
<td>23°C/65°C</td>
<td>133 kPa/ 133 kPa</td>
</tr>
<tr>
<td>HX 2</td>
<td>Heat exchanger</td>
<td>199.07 kW</td>
<td>23°C/82°C</td>
<td>133 kPa/ 133 kPa</td>
</tr>
<tr>
<td>HX 3</td>
<td>Heat exchanger</td>
<td>15.925 kW</td>
<td>71°C/23°C</td>
<td>133 kPa/ 133 kPa</td>
</tr>
<tr>
<td>C1</td>
<td>Condenser</td>
<td>9.87 kW</td>
<td>75°C/65°C</td>
<td>133 kPa/ 133 kPa</td>
</tr>
<tr>
<td>M1</td>
<td>Joint</td>
<td>N/A</td>
<td>23°C/23°C</td>
<td>133 kPa/ 133 kPa</td>
</tr>
<tr>
<td>M2</td>
<td>Joint</td>
<td>N/A</td>
<td>65°C/65°C</td>
<td>133 kPa/ 133 kPa</td>
</tr>
<tr>
<td>M3</td>
<td>Joint</td>
<td>N/A</td>
<td>65°C/65°C</td>
<td>133 kPa/ 133 kPa</td>
</tr>
<tr>
<td>DU</td>
<td>Devolatilization Unit</td>
<td>N/A</td>
<td>65°C/65°C</td>
<td>133 kPa/ 133 kPa</td>
</tr>
<tr>
<td>DC</td>
<td>Distillation Column</td>
<td>Cond. 2127 MJ/hr Reboil. 2093 MJ/hr</td>
<td>Inlet 75°C Outlet 71°C/110°C</td>
<td>133 kPa/ 133 kPa</td>
</tr>
</tbody>
</table>

Table 2: This table shows the duties, inlet and outlet temperatures, and pressures of the unit ops.
<table>
<thead>
<tr>
<th>Stream Number</th>
<th>Flowrates (( \frac{kg}{hr} ))</th>
<th>Stream Number</th>
<th>Flowrates (( \frac{kg}{hr} ))</th>
</tr>
</thead>
<tbody>
<tr>
<td>F1</td>
<td>AIBN- 182.4358</td>
<td>S6</td>
<td>Methanol- 532</td>
</tr>
<tr>
<td>F2</td>
<td>Methanol- 1838.69</td>
<td>S7</td>
<td>Nitrogen- 13.048</td>
</tr>
<tr>
<td>F3</td>
<td>VAM- 5567.392</td>
<td>S8</td>
<td>PVAc- 5531.616</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>VAM- 35.778</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Methanol- 2386.025</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>AIBN- 72.974</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Hydroquinone- 0.056951</td>
</tr>
<tr>
<td>F4</td>
<td>Hydroquinone- 0.056951</td>
<td>S9</td>
<td>PVAc- 35.778</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Methanol- 547.335</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>AIBN- 72.974</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Hydroquinone- 0.056951</td>
</tr>
<tr>
<td>F5</td>
<td>Methanol- 532</td>
<td>S10</td>
<td>PVAc- 5531.616</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Methanol- 2370.69</td>
</tr>
<tr>
<td>S1</td>
<td>Methanol- 1838.69 AIBN- 182.4358</td>
<td>S12</td>
<td>AIBN- 72.974</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Hydroquinone- 0.056951</td>
</tr>
<tr>
<td>S2</td>
<td>VAM- 5567.392 Methanol- 1838.69</td>
<td>S15</td>
<td>Methanol- 547.335</td>
</tr>
<tr>
<td></td>
<td>AIBN- 182.4358</td>
<td></td>
<td>VAM- 35.778</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Methanol- 2386.025</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>AIBN- 72.974</td>
</tr>
<tr>
<td>S5</td>
<td>Methanol- 79.152 Nitrogen- 13.048</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 3: This table shows the flow rates of each stream represented in the flowsheet, excluding the utility streams.

**Land Acquisition:**

Many configurations were considered in the overall design of the Mantis Polymers plant in Baton Rouge, Louisiana. Mantis Polymers decided on a location south of Baton Rouge in a region known as Carville, Louisiana. It will be situated on a 25 acre plot on the Mississippi River for the purpose of shipping and receiving goods by barge. The price of this waterfront property is $45,000 per acre, which amounts to $1.1 million dollars. Mantis Polymers believes this location would be advantageous due to the close proximity of Methanex and Dow Chemical, the primary suppliers of methanol and VAM. The railroad is also a plausible resource for shipping and receiving due to its close proximity to the plant; however, shipment by barge is preferred. The cost by weight to transport chemicals by railroad is $0.04 per ton mile; the cost by barge is $0.0066 per ton mile.
Figure 1: Proposed location of production plant

**Selling Price of Polyvinyl Acetate**

Due to an update in market information from phase I, the cost analysis will be based on a selling price of $2000/US ton for polyvinyl acetate. This value is more representative of the true selling price based on market trends and forecasting. The previous selling price of $2500/US ton yielded an excessive, unrealistic profit. This overestimation would have been disastrous, considering the magnitude of this proposed production plant design. Using a lower selling price value provides space for potential growth with the market. All necessary expenses to produce a correct quantity of product that meets all consumer specifications are factored into the decision-point.
Cost Analysis:

<table>
<thead>
<tr>
<th></th>
<th>Net (after-tax) Profit Total</th>
<th>Total Capital Investment</th>
<th>Return on Investment</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$8,283,999.26</td>
<td>$19,353,764.14</td>
<td>43%</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Installed Cost of Heat exchangers</th>
<th>Operating Costs</th>
</tr>
</thead>
<tbody>
<tr>
<td>HX1</td>
<td>$41,588.99</td>
</tr>
<tr>
<td>HX2</td>
<td>$44,170.10</td>
</tr>
<tr>
<td>HX3</td>
<td>$10,158.18</td>
</tr>
<tr>
<td>C1</td>
<td>$5,857.98</td>
</tr>
<tr>
<td>Total</td>
<td>$101,775.25</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Installed Cost of Pumps w/ Motor</th>
<th>Operating Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>P1</td>
<td>$4,757.08</td>
</tr>
<tr>
<td>P2</td>
<td>$6,376.93</td>
</tr>
<tr>
<td>P3</td>
<td>$6,868.49</td>
</tr>
<tr>
<td>P4</td>
<td>$4,002.91</td>
</tr>
<tr>
<td>P5</td>
<td>$4,154.40</td>
</tr>
<tr>
<td>Total</td>
<td>$26,159.80</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Installed Cost of Reactor</th>
<th>Operating Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1 w/ agitator</td>
<td>$761,648.94</td>
</tr>
<tr>
<td>Total</td>
<td>$761,648.94</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Installed Cost of Devolatilization</th>
<th>Operating Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>


### Installed Cost of Distillation Column | Operating Cost

<table>
<thead>
<tr>
<th></th>
<th>Unit</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>DC</td>
<td>DU</td>
<td>$877,444.52</td>
<td>$123.37</td>
</tr>
<tr>
<td>Total</td>
<td>$877,444.52</td>
<td>$123.37</td>
<td></td>
</tr>
</tbody>
</table>

### Installed Cost of Agitator | Operating Cost

<table>
<thead>
<tr>
<th></th>
<th>Unit</th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>A1</td>
<td>DU</td>
<td>$70,638.27</td>
<td>$14,524.95</td>
</tr>
<tr>
<td>Total</td>
<td>$70,638.27</td>
<td>$14,524.95</td>
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</tr>
</tbody>
</table>

### Total Bare Module Cost:

<table>
<thead>
<tr>
<th>Description</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost of Fabricated Equipment</td>
<td>$3,096,492.76</td>
</tr>
<tr>
<td>Cost of Process Machinery</td>
<td>$26,159.80</td>
</tr>
<tr>
<td>Cost of Spare(Pump, Valves, Comps)</td>
<td>$154,559</td>
</tr>
<tr>
<td>Cost of Storage Tanks</td>
<td>$61,823.70</td>
</tr>
<tr>
<td>Cost of Startup Equipment</td>
<td>$92,735.50</td>
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</tbody>
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\[ C_{TBM} = 3,306,301.84 \]

### Direct Permanent Investment Cost:

<table>
<thead>
<tr>
<th>Description</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost of Total Bare Module</td>
<td>$3,306,301.84</td>
</tr>
<tr>
<td>Cost of Site Preparation</td>
<td>$113,608.00</td>
</tr>
<tr>
<td>Service Facilities</td>
<td>$686,460.37</td>
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<tr>
<td>Cost of Allocation/Utilities</td>
<td>$380,985.50</td>
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\[ C_{DPI} = 4,613,355.28 \]
<table>
<thead>
<tr>
<th>Total Depreciable Capital:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost of Direct Permanent Investment</td>
</tr>
<tr>
<td>Cost of Contingencies</td>
</tr>
<tr>
<td>Cost of Contractor Fees</td>
</tr>
<tr>
<td>$C_{TDC}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Total Permanent Investment:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cost of Total Depreciation Capital</td>
</tr>
<tr>
<td>Cost of Land</td>
</tr>
<tr>
<td>Cost of Royalties</td>
</tr>
<tr>
<td>Startup Costs(New Process)</td>
</tr>
<tr>
<td>$C_{TPI}$</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Investment Site Factors:</th>
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</thead>
<tbody>
<tr>
<td>Total Permanent Investment Cost</td>
</tr>
<tr>
<td>Investment Site Factor</td>
</tr>
<tr>
<td>$C^*_{TPI}$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Total Capital Investment:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Permanent Investment</td>
</tr>
<tr>
<td>Working Capital Cost</td>
</tr>
<tr>
<td>$C_{TCI}$</td>
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</table>

<table>
<thead>
<tr>
<th>Sales Revenue:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Polymer Sell Price</td>
</tr>
<tr>
<td>Total Polymer Sell Price:</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Cost of Feedstocks:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed of AIBN</td>
</tr>
<tr>
<td>$C_{Feedstock}$</td>
</tr>
<tr>
<td>Feed of Methanol</td>
</tr>
<tr>
<td>$C_{Feedstock}$</td>
</tr>
<tr>
<td>Feed of Hydroquinone</td>
</tr>
<tr>
<td>$C_{Feedstock}$</td>
</tr>
<tr>
<td>Feed of Vinyl Acetate</td>
</tr>
<tr>
<td>$C_{Feedstock}$</td>
</tr>
<tr>
<td>$C_{Feedstock}$</td>
</tr>
</tbody>
</table>
### Cost of Utilities:

<table>
<thead>
<tr>
<th>Service</th>
<th>Quantity/Description</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cooling Utilities</td>
<td>271,580 m³ at $0.03/m³</td>
<td>$8,147.40</td>
</tr>
<tr>
<td>Heating Utilities</td>
<td>57,572.70 m³ at $0.5/m³</td>
<td>$2,878.64</td>
</tr>
<tr>
<td>Steam Utilities</td>
<td>242,590.33 tons at $6.6/ton</td>
<td>$1,601,096.18</td>
</tr>
<tr>
<td>Electricity</td>
<td>843,288 kW-hr at $0.0642/kW-hr</td>
<td>$54,139.09</td>
</tr>
<tr>
<td>Wastewater Treatment</td>
<td>195,947 kg at $0.33/kg</td>
<td>$195,946.87</td>
</tr>
</tbody>
</table>

\[ C_{\text{Util}} = \$1,862,208.18 \]

### Cost of Manufacturing:

<table>
<thead>
<tr>
<th>Description</th>
<th>Details</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Work Hours</td>
<td>40 hr/week x 52 weeks</td>
<td>2080 hrs</td>
</tr>
<tr>
<td>Cost per Operator</td>
<td>$50/hr</td>
<td></td>
</tr>
<tr>
<td>Number of Shifts</td>
<td>8200 hr/ work hours</td>
<td>3.942~4.00 shifts</td>
</tr>
<tr>
<td>Number of Operators</td>
<td>24 Operators/4 shifts</td>
<td>4 operators/shift</td>
</tr>
<tr>
<td>DW&amp;B</td>
<td></td>
<td>$2,460,000/yr</td>
</tr>
<tr>
<td>SDW&amp;B</td>
<td>0.15*DW&amp;B</td>
<td>$369,000.00/yr</td>
</tr>
<tr>
<td>Tech Assistance</td>
<td>$60,000/yr at 1 person</td>
<td>$60,000.00/yr</td>
</tr>
<tr>
<td>Control Lab</td>
<td>$60,000/yr at 2 persons</td>
<td>$120,000.00/yr</td>
</tr>
<tr>
<td>Supplies and Services</td>
<td>0.06*DW&amp;B</td>
<td>$147,600.00/yr</td>
</tr>
</tbody>
</table>

\[ C_{\text{Op}} = \$3,156,600.00/yr \]

### Cost of Maintenance:

<table>
<thead>
<tr>
<th>Description</th>
<th>Details</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Depreciable Capital</td>
<td></td>
<td>$5,905,094.75</td>
</tr>
<tr>
<td>MW&amp;B</td>
<td>0.045*C_{\text{TDC}}(\text{Solid-Liq})</td>
<td>$265,729.26</td>
</tr>
<tr>
<td>SMW&amp;B</td>
<td>0.25*MW&amp;B</td>
<td>$66,432.32</td>
</tr>
</tbody>
</table>

\[ C_{\text{Maint}} = \$611,177.31 \]

### Cost of Manufacturing: Operation Overhead

<table>
<thead>
<tr>
<th>Description</th>
<th>Formula</th>
<th>Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>M&amp;O SW&amp;B</td>
<td>DW&amp;B+SDW&amp;B+MW&amp;B+SMW&amp;B</td>
<td>$3,161,161.58</td>
</tr>
<tr>
<td>General Plant Overhead</td>
<td>0.071*M&amp;O SW&amp;B</td>
<td>$224,442.47</td>
</tr>
<tr>
<td>Mechanical Department</td>
<td>0.024*M&amp;O SW&amp;B</td>
<td>$75,867.88</td>
</tr>
<tr>
<td>Employee Relations Department</td>
<td>0.024*M&amp;O SW&amp;B</td>
<td>$75,867.88</td>
</tr>
<tr>
<td>Business Services</td>
<td>0.074*M&amp;O_SW&amp;B</td>
<td>$233925.96</td>
</tr>
<tr>
<td>-------------------</td>
<td>---------------</td>
<td>------------</td>
</tr>
<tr>
<td></td>
<td><strong>C_{Ov}</strong></td>
<td>$610,104.19</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Cost of Operations: Taxes, Insurance, and Depreciation</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>C_{TDC}</strong></td>
</tr>
<tr>
<td><strong>C_{Alloc}</strong></td>
</tr>
<tr>
<td><strong>C_{T&amp;I}</strong></td>
</tr>
<tr>
<td><strong>Depreciation (direct plant onsite)</strong></td>
</tr>
<tr>
<td><strong>Depreciation (Allocated plant offsite)</strong></td>
</tr>
<tr>
<td><strong>C_{Dep}</strong></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>COM: Cost of Manufacture</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>C_{Feedstocks}</strong></td>
</tr>
<tr>
<td><strong>C_{Util}</strong></td>
</tr>
<tr>
<td><strong>C_{Op}</strong></td>
</tr>
<tr>
<td><strong>C_{Maint}</strong></td>
</tr>
<tr>
<td><strong>C_{Ov}</strong></td>
</tr>
<tr>
<td><strong>C_{T&amp;I}</strong></td>
</tr>
<tr>
<td><strong>C_{Dep}</strong></td>
</tr>
<tr>
<td><strong>COM</strong></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Costs: General Expenses</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>COM</strong></td>
</tr>
<tr>
<td><strong>GE</strong></td>
</tr>
<tr>
<td><strong>C</strong></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Working Capital</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Cash Reserves</strong></td>
</tr>
<tr>
<td><strong>Inventory</strong></td>
</tr>
<tr>
<td><strong>Accounts Receivable</strong></td>
</tr>
<tr>
<td><strong>Accounts Payable</strong></td>
</tr>
<tr>
<td><strong>C_{WC}</strong></td>
</tr>
</tbody>
</table>
### Gross and After Tax Earnings:

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Annual sale Revenue (S)</td>
<td>$50,000ton/yr x $2,500/ton</td>
<td>$100,000,000.00</td>
</tr>
<tr>
<td>Annual Product Cost (C)</td>
<td>COMGE</td>
<td>$86,850,794.82</td>
</tr>
<tr>
<td>Gross (pre-tax) Earnings (GPT)</td>
<td>S-C</td>
<td>$13,149,205.18</td>
</tr>
<tr>
<td>Net (after-tax) Earnings (NPT)</td>
<td>0.63*GPT</td>
<td>$8,283,999.26</td>
</tr>
</tbody>
</table>

### Profitability:

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Return on Investment (ROI)</td>
<td>NPT/C_{TCI}</td>
<td>0.428</td>
</tr>
<tr>
<td>Pay Back Period (PBP)</td>
<td>C_{TDC}/(NPT+C_{Dep})</td>
<td>0.675</td>
</tr>
<tr>
<td>Venture Profit (VP)</td>
<td>NPT-0.02*C_{TCI}</td>
<td>$7,800,155.16</td>
</tr>
<tr>
<td>Risk Assessment</td>
<td>Slightly High</td>
<td>25%</td>
</tr>
</tbody>
</table>

As it stands, Mantis Polymers believes that the values provided above are accurate estimate of the costs required for a continuous, solution polymerization plant. Due to the complexity of some of the unit op components such as the devolatilization unit and reactor, the overall cost was doubled. Mantis’ justification for doubling the reactor’s cost is that it can incorporate the cooling jacket construction and added support for the weight of the overall system. Also, until an official price estimate from the supplier is provided, the overall cost of the devolatilization unit calculated should be doubled due to the complexity of its separation system.

**Recommendations:**

With a net (after tax) profit total of **$8,284,000.00** and a total capital investment of **$19,354,000**, Mantis has determined that the return on investment (ROI) for this facility would be 43%. However, the venture of solution polymerization was found to be slightly high at 25% risk. This is due to industry having knowledge of polymerization of vinyl acetate, but using emulsion to produce the polymer. Nonetheless, this process was found to be feasible according to Mantis Polymers Corporate requirements and would like to begin construction of the facility.
References:

PVAc:

Hydroquinone:
Appendix A

Nomenclature

\( a_1 \) pump cost coefficients
\( a_2 \) pump cost coefficients
\( a_3 \) pump cost coefficients
\( HP \) Horsepower of Motors
\( C_m \) Cost of motor
\( b_1 \) pump cost coefficients
\( b_2 \) pump cost coefficients
\( b_3 \) pump cost coefficients
\( F \) material coefficient
\( Q \) flow rate
\( H \) head
\( S \) size factor
\( F_T \) size factor coefficient
\( C_b \) bare cost
\( \eta \) pump efficiency
\( P_s \) shaft power
\( C_{\text{Installed}} \) cost of instillation
\( P_B \) brake power
\( \alpha \) energy per year
\( C_{\text{Installed with motor}} \) cost of installed pump with motor
\( C_{\text{op}} \) operating cost
\( T \) thickness
\( D \) diameter
\( L \) length
\( A \) surface area
\( \rho_{\text{steel}} \) density of steel
\( W \) weight
\( V \) volume
\( W \rho_{\text{Metal}} \) material density
\( F_M \) material coefficient
\( C_v \) vertical vessel coefficient
\( C_b \) vertical vessel coefficient
\( C_{bm} \) bare module cost
\( \text{Cooling water cost} \) cost of cooling water
\( D_{\text{Reactor}} \) diameter of reactor
\( H_{\text{Reactor}} \) height of reactor
\( \text{jacket} \) diameter of jacket
\( D_{\text{jacket}} \) diameter of reactor with jacket
\( V_{\text{Vol Reactor}} \) volume of reactor

\( \text{Tot}_{\text{Volume per year}} \) total volume per year
\( \text{Cost} \) operating cost of reactor
\( \rho_{\text{VAM}} \) density of VAM
\( \rho_{\text{Methanol}} \) density of methanol
\( \rho_{\text{AIBN}} \) density of AIBN
\( \rho_{\text{Hydroquinone}} \) density of hydroquinone
\( \rho_{\text{PVAc}} \) density of PVAc
\( L_1 \) devolatilizer length
\( V_1 \) devolatilizer volume
\( D_1 \) devolatilizer diameter
\( h_1 \) devolatilizer height
\( r_1 \) devolatilizer radius
\( S.A. \) surface area of a cylinder
\( S.A.1 \) devolatilizer surface area
\( V_{1,\text{shell}} \) devolatilizer shell volume
\( \rho_{\text{S.S.316}} \) density of stainless steel 316
\( W_1 \) devolatilizer weight
\( Q_1 \) heat exchanger duty
\( Q_1 \) pump cost coefficients
\( U_0 \) overall heat transfer coefficient
\( T_{LM} \) log mean temperature difference
\( A \) area of heat exchange
\( F_d \) heat exchanger area factor
\( L_{\text{Column}} \) distillation column length
\( D_{\text{Column}} \) distillation column diameter
\( \rho_{\text{Metal}} \) material density
\( N_{\text{Trays}} \) number of trays
\( \text{Thickness} \) distillation column thickness
\( V_1 \) distillation column volume
\( V_{\text{Shell}} \) volume of column shell
\( \text{Weight}_{\text{Column}} \) weight of distillation column
\( f_1 \) column material factor
\( f_2 \) column diameter coefficient
\( f_3 \) tray type factor
\( C_{P1} \) cost of platforms and ladders
\(Vol_{Jacket}\) volume of jacket
\(\Delta V\) difference in volume of reactor and jacket
\(C_{T1}\) cost of trays
\(C_{T2}\) tower cost
\(C_{Tot}\) total cost of column
\(\text{Cooling}_C\) cooling water cost
\(\text{Duty}\) duty of column condenser
\(C_p\) specific heat capacity
\(dT\) temperature difference condenser
\(\text{mass}\) water mass per hour
\(M_{year}\) water mass per year
\(\rho\) density of water
\(Q_{Duty}\) duty of column reboiler
\(\Delta T\) temperature difference reboiler
\(mdot\) mass flowrate of steam
\(C_{steam}\) cost per kilogram of steam
\(N_{op/yea}\) annual hours of operation
\(C_{op/rebo}\) operating cost of reboiler
\(C_{Pumps}\) bare module cost of pumps
\(C_{Reactor}\) bare module cost of reactor
\(C_{Dist}\_Col\) bare module column cost
\(C_{agitation}\) bare module agitator cost
\(C_{Hex}\) bare module cost of heat exchangers
\(C_{Dev}\) bare module devolatilizer cost
\(C_{FE}\) total equipment bare module cost
\(C_{PM}\) total machinery bare module cost
\(C_{Spare}\) total spare bare module cost
\(C_{Storage}\) total storage tanks bare module cost
\(C_{Startup}\) total equipment startup cost
\(C_{TBM}\) total bare module investment
\(C_{land}\) cost of land
\(C_{Site}\) cost of site preparation
\(C_{Serv}\) cost of service facilities
\(C_{Utility}\) cost of utilities
\(C_{MPI}\) cost of direct permanent investment
\(C_{Cont}\) cost of contingencies and contractors fees
\(C_{TDC}\) total depreciable capital
\(C_{Royal}\) cost of royalties
\(\text{TPI}\) total permanent investment
\(F_{ISF}\) investment site factor
\(\text{TPI}\_\text{star}\) total permanent investment with site
\(C_{WC}\) working capital
\(P_{\text{Polymer}}\) polymer production tons per year
\(F_{\text{Hydroquinone}}\) feedstock of hydroquinone
\(F_{\text{VAM}}\) feedstock of VAM
\(C_{\text{AIBN}}\) cost of AIBN
\(C_{\text{VAM}}\) cost of VAM
\(C_{\text{Methanol}}\) cost of methanol
\(C_{\text{Feedstocks}}\) total cost of feedstocks
\(\Sigma_{\text{Cooling}_\text{Utilities}}\) total cost of cooling utilities
\(\Sigma_{\text{Steam}_\text{Utilities}}\) total cost of steam utilities
\(\Sigma_{\text{Heating}_\text{Utilities}}\) total cost of heating utilities
\(\Sigma_{\text{Electricity}}\) total cost of electricity utilities
\(\Sigma_{\text{Waste}}\) total cost of waste removal
\(C_{\text{Util}}\) total cost of all utilities
\(C_{\text{FEU}}\) total cost of feedstocks and utilities
\(\text{workhours}\) labor hours per year
\(N_{\text{Shifts}}\) number of shifts
\(N_{\text{Ops}}\) number of operators
\(D\_\text{W}\_\text{B}\) direct wages and benefits
\(SD\_\text{W}\_\text{B}\) salaries, direct wages, benefits
\(\text{Control}_\text{Lab}\) cost of control lab
\(C_{\text{Op}}\) labor-related operational costs
\(M\_\text{W}\_\text{B}\) maintenance, wages, benefits
\(C_{\text{Maint}}\) cost of maintenance
\(\text{SM}\_\text{W}\_\text{B}\) salaries, maintenance, wages, benefits
\(M\&O\_\text{SW}\_\text{B}\) maintenance and labor
\(\text{Gen}_\text{Plant}_\text{Overhead}\) plant overhead
\(\text{Mech}_\text{Dept}\) mechanical department services
\(\text{Emp}_\text{Rel}_\text{Dept}\) employee relations department
\(\text{Bus}_\text{Services}\) business services
\(C_{\text{OV}}\) overhead cost
\(C_{\text{Alloc}}\) allocated plant (offsite)
\(C_{\text{T&I}}\) taxes and insurance
\(D\_\text{PO}\) direct plant onsite
\(D\_\text{AP}\) allocated plant (offsite)
\(C_{\text{Dep}}\) depreciation
\(C_{\text{Feedstocks}}\) cost of feedstocks
\(C_{\text{Op}}\) cost of operations
\(C_{\text{OV}}\) cost of overhead
\(C_{\text{Dep}}\) cost of depreciation
\begin{itemize}
\item $C_{\text{Util}}$ cost of utilities
\item $C_{\text{Polymer}}$ polymer cost per year
\item $C_{\text{Maint}}$ cost of maintenance
\item $F_{\text{AIBN}}$ feedstock of AIBN
\item $F_{\text{Methanol}}$ feedstock of methanol
\item $C_{\text{T\&I}}$ cost of taxes and insurance
\item COM cost of manufacturing
\item GE central operations
\item C general expenses
\item CR cash reserves
\item Inv inventories
\item AcctPay accounts payable
\item AcctRec accounts receivable
\item $C_{\text{WC}}$ working capital
\item S annual sales revenue
\item C annual product cost
\item GPT gross pre-tax earnings
\item NPT net after-tax earnings
\item ROI return on investment
\item PBP payback period
\item VP venture profit
\item $C_A$ annualized cost
\item $i_m$ return on investment of deposits
\end{itemize}
Appendix B

Sample Calculations for Phase III: Mantis

Pump 2 Motor Costs:

\[
a_1 := 5.4166 \quad a_2 := 0.31216 \quad a_3 := 0.10573
\]

\[
HP := 0.25
\]

\[
Cm := 2.20 \times e^{\left(a_1 + a_2 \cdot \ln(HP) + a_3 \cdot \left(\ln(HP)^2\right)\right)} = 393.667 \text{ $}
\]

Pump 2 Costs:
Centrifugal prices in $:
Variables defined below for the pumps.

\[ F := 1.0 \quad b_1 := 5.1029 \quad b_2 := -1.2217 \quad b_3 := 0.0771 \]

\[ Q := 26.2 \quad H := 11.4 \quad S := Q \cdot (H)^{0.5} = 88.461 \]

Pump cost equations are shown below for the first pump. The cost is multiplied by the \( F_m \), \( F_T \), \( C_b \). The cost is then added to the cost of the motor to give the total costs.

\[ F_T := e^{\left(b_1 + b_2 \cdot \left(ln(Q \cdot \sqrt{H})\right) + b_3 \cdot (ln(S))^3\right)} = 3.241 \]

\[ C_b := 1407 \cdot F \cdot Q^{0.52} = 7687.954 \text{ $} \]

\[ \eta := 0.65 \quad P_S := 0.027775 \text{ kW} \]

\[ C_{\text{Installed}} := 1.4 \cdot C_b = 10763.135 \text{ $} \quad 1.4 \text{ Stainless steel multiplier} \]

\[ P_B := \frac{P_S}{\eta} = 42.731 \text{ W} \quad A := 8200 \text{ hr} \cdot P_B \quad \text{Cost} := 0.0642 \frac{\text{ $}}{\text{kW} \cdot \text{hr}} \]

\[ C_{\text{Installed with motor}} := C_{\text{Installed}} + Cm = 1156.802 \text{ $} \quad \text{Total cost of P2.} \]

\[ C_{\text{op}} := A \cdot \text{Cost} = 22.495 \text{ $/year} \]
Cost of Agitator (AIBN)

\[ HP := 37 \quad a := 9.25 \quad b := 0.2801 \quad c := 0.0542 \]

\[ C := 1.218 \times e^{\left( a + b \times \ln(HP) + c \times (\ln(HP))^2 \right)} = 70638.27 \text{ $} \]

Operating Costs:

\[ HP := 37 \quad hp = 27.591 \text{ kW} \]

\[ C_{Op} := HP \times 8200 \times \frac{hr}{yr} \times 0.0642 \times \frac{\text{ $}}{kW \cdot hr} = 14524.951 \times \frac{\text{ $}}{yr} \]

Cost of Agitator (Reactor)

\[ HP := 50 \quad a := 9.25 \quad b := 0.2801 \quad c := 0.0542 \]

\[ C := 1.218 \times e^{\left( a + b \times \ln(HP) + c \times (\ln(HP))^2 \right)} = 86893.672 \text{ $} \]

Operating Costs:

\[ HP := 50 \quad hp = 37.285 \text{ kW} \]

\[ C_{Op} := HP \times 8200 \times \frac{hr}{yr} \times 0.0642 \times \frac{\text{ $}}{kW \cdot hr} = 19628.312 \times \frac{\text{ $}}{yr} \]

Pressure Vessel (Reactor)

Vertical

Dimensions of the Polymer reactor.

\[ T := 1.15 \text{ in} \quad D := 9.6104 \text{ ft} \quad L := 19.68 \text{ ft} \]
\[ D = 2.929 \text{ m} \quad L = 5.998 \text{ m} \]

Surface area calculation to determine the weight of the polymer reactor.

\[ A := 2 \times \pi \times \frac{D}{2} \times L + 2 \pi \times \left( \frac{D}{2} \right)^2 \]
\[ \rho_{steel} := 500 \frac{lb}{ft^3} \]
\[ V := A \times T = 70.845 \text{ ft}^3 \]
\[ W := V \times \rho_{steel} = 35422.694 \text{ lb} \]
\[ W = 35422.694 \text{ lb} \]
The weight of the pressure vessel will be doubled to take into account the cooling jacket of the reactor.

\[ W := 2 \cdot W = 70845.389 \text{ lb} \]

Values restated without units to calculate the bare module cost.

\[
F_M := 2.1 \quad W := W \cdot \frac{1}{\text{lb}} \quad D := 9.6104 \quad L := 19.68
\]

\[
C_a := 480 \cdot D^{0.7396} \cdot L^{0.7066} = 21010.431 \text{ \$}
\]

\[
C_b := 1.672 \cdot e^{(9.100 - 0.2889 \cdot (\ln(W)) + 0.04576 \cdot (\ln(W))^4)} = 179002.113 \text{ \$}
\]

\[
C_{bm} := F_M \cdot C_b + C_a = 396914.9 \text{ \$}
\]

\[
C_{\text{Installed}} := 1.7 \cdot C_{bm} = 674755.274 \text{ \$} \quad \text{1.7 multiplier for a stainless steel pressure vessel.}
\]

Operational Costs of the Reactor are shown below.

\[
\text{Cooling Water Cost} := 0.03 \frac{\text{\$}}{\text{m}^3} \quad D_{\text{Reactor}} := 2.929 \text{ m} \quad H_{\text{Reactor}} := 5.998 \text{ m}
\]

\[
\text{jacket} := 0.5 \text{ m}
\]

\[
D_{\text{Jacket}} := D_{\text{Reactor}} + \text{jacket} = 3.429 \text{ m} \quad H_{\text{Jacket}} := 5.998 \text{ m}
\]

\[
\text{Vol}_{\text{Reactor}} := 36.372 \text{ m}^3 \quad \text{Vol}_{\text{Jacket}} := 49.851 \text{ m}^3
\]

\[
\Delta V := \text{Vol}_{\text{Jacket}} - \text{Vol}_{\text{Reactor}} = 13.479 \text{ m}^3
\]

\[
\text{Tot Volume per year} := \Delta V \cdot 8200 = 110527.8 \text{ m}^3
\]

\[
\text{Cost} := \text{Tot Volume per year} \cdot \text{Cooling Water Cost} = 3315.834 \text{ \$}
\]

Pressure Vessel(Devolatilizer)

\[
\rho_{VAM} := 1100 \frac{\text{kg}}{\text{m}^3} \quad \rho_{\text{Methanol}} := 1100 \frac{\text{kg}}{\text{m}^3} \quad \rho_{\text{AIBN}} := 1100 \frac{\text{kg}}{\text{m}^3}
\]
\( \rho_{\text{Hydroquinone}} := 1100 \frac{kg}{m^3} \quad \rho_{\text{PVAc}} := 1100 \frac{kg}{m^3} \)

Total solution going into the devolatilizer is \(9.0345 \text{ m}^3/\text{hr}\)

\[
L_1 := 4 \text{ m} \quad V_1 := 18.22678 \text{ m}^3 \quad D_1 := \sqrt{\frac{V_1 \cdot 4}{\pi \cdot L_1}} = 7.903 \text{ ft} \quad D_1 = 2.409 \text{ m}
\]

\[
h_1 := L_1 = 13.123 \text{ ft} \quad r_1 := 0.5 \cdot D_1 = 3.951 \text{ ft}
\]

\[
S.A. = 2 \pi r h + 2 \pi r^2
\]

\[
S.A.1 := 2 \pi r_1 h_1 + 2 \pi r_1^2 = 423.902 \text{ ft}^2
\]

\[
t_{\text{SS316}} := 1.15 \text{ in} = 0.09583 \text{ ft}
\]

\[
V_{1,\text{shell}} := S.A.1 \cdot t_{\text{SS316}} = 40.624 \text{ ft}^3
\]

\[
\rho_{\text{S.S.316}} := 500 \frac{lb}{\text{ft}^3}
\]

\[
W_1 := V_{1,\text{shell}} \cdot \rho_{\text{S.S.316}} = 9213.363 \text{ kg}
\]

\[
W_1 := V_{1,\text{shell}} \cdot \rho_{\text{SS.316}} = 20311.989 \text{ lb}
\]

A horizontal pressure vessel will be used due to the weight range allowed

\[
C = F_M \cdot C_b + C_a
\]

\[
D_1 := 5.564 \quad F_M := 2.1 \quad W_1 := 40623.979
\]

\[
C_{a1} := 2291 \cdot D_1^{0.2029} = 3245.369 \text{ $}
\]

\[
C_{b1} := 1.672 \cdot e^{(8.571 - 0.2330 \cdot \ln(W_1) + 0.04333 \cdot (\ln(W_1))^2)} = 97938.091 \text{ $}
\]
\[ C_1 := F_M \cdot C_{b1} + C_{a1} = 208915.361 \text{ $} \] Cost for the vessel ($)

**Multiply the cost of the vessel by the Instillation cost multiplier for S.S. 316**

\[ F_{I.multiplier} := 2.1 \]

\[ C_{1.Total} := C_1 \cdot F_{I.multiplier} = 438722.259 \text{ $} \]

The team decided that a multiplication factor of 2 would adequately and accurately represent the cost of a Devolatization unit.

\[ C_{Total} := 2 \cdot C_{1.Total} = 877444.517 \text{ $} \]

**Operational Cost of the devolatizer.**

The cost to operate the devolatizer was taken into account in the heat exchanger heating methanol up to vapor and a Condenser on the downstream side.

**Cost of Heat exchanger 1:**

**Floating Head**

\[ Q_1 := 185.517 \frac{BTU}{s} \quad U_0 := 0.015 \frac{BTU}{s \cdot ft^2 \cdot F} \quad T_{LM} := 44.9520 \text{ F} \]

\[ A := \frac{Q_1}{U_0 \cdot T_{LM}} = 275.133 \text{ ft}^2 \quad A := 275.1335 \]

\[ C_b := $ \cdot e^{(11.667 - 0.8709 \cdot \ln (A) + 0.09 \cdot (\ln (A))^2)} = 14984.216 \text{ $} \]

\[ F_d := e^{(-1.1156 + 0.0906 \cdot \ln (A))} = 0.545 \quad \text{Fixed Head:} \]

\[ F_m := 2.2 F_p := 1 \]

\[ C_{bm} := 1.218 \cdot F_p \cdot F_m \cdot F_d \cdot C_b = 21889.09 \text{ $} \]

\[ C_{Installed} := 1.9 \cdot C_{bm} = 41589.271 \text{ $} \]

-For shell and tube stainless steel heat exchanger the multiplier is 1.9.
Operational cost of HX 1.

\[ m_{dot} := 4000 \, \text{kg/hr} \]
\[ \rho_{\text{water}} := 997 \, \text{kg/m}^3 \]
\[ t := 8200 \, \text{hr} \]
\[ C_{\text{water}} := 0.50 \, \$/m^3 \]

\[ C_{\text{heat Util}} := \frac{m_{dot} \cdot t \cdot C_{\text{water}}}{\rho_{\text{water}}} = 16449.348 \, \$ \]

Cost of Distillation Column:

\[ L_{\text{Column}} := 50 \, \text{ft} \]
\[ D_{\text{Column}} := 8 \, \text{ft} \]
\[ \rho_{\text{Metal}} := 500 \, \text{lb/ft}^3 \]
\[ D_{\text{Column}} = 2.438 \, \text{m} \]
\[ N_{\text{Trays}} := 23 \]
\[ F_M := 3.0 \]
\[ \text{Thickness} := 0.75 \, \text{in} \]

\[ V1 := \frac{\pi}{4} \cdot D_{\text{Column}}^2 \cdot L_{\text{Column}} = 2513.274 \, \text{ft}^3 \]

\[ V2 := \frac{\pi}{4} \cdot (D_{\text{Column}} + 2 \cdot \text{Thickness})^2 \cdot L_{\text{Column}} = 2592.428 \, \text{ft}^3 \]

\[ V_{\text{Shell}} := V2 - V1 = 79.153 \, \text{ft}^3 \]

\[ Vol_{\text{Column}} := V_{\text{Shell}} \]

\[ Weight_{\text{Column}} := Vol_{\text{Column}} \cdot \rho_{\text{Metal}} = 39576.704 \, \text{lb} \]
\[ W := Weight_{\text{Column}} \cdot \frac{1}{\text{lb}} = 39576.704 \]

\[ f_1 := 2.1 \]
\[ f_2 := 1.401 + \frac{0.0724}{\text{ft}} \cdot D_{\text{Column}} = 1.98 \]
\[ f_3 := 1.0 \]

\[ Ratio := \frac{L_{\text{Column}}}{D_{\text{Column}}} = 6.25 \]

\[ C_b := 1.218 \cdot e^{(7.123 + 0.1478 \cdot \ln(W) + 0.92488 \cdot \ln(W)^2 + 0.0158 \cdot Ratio \cdot \ln(1))} = 117354.615 \]

\[ D_{\text{Column}} := 8 \]
\[ L_{\text{Column}} := 50 \]
\[ C_{P1} := 249.6 \cdot D_{\text{Column}}^{0.6332} \cdot L_{\text{Column}}^{0.8016} = 21427.698 \]

\[ C_{T1} := 457.7 \cdot e^{(0.1739 \cdot D_{\text{Column}})} = 1839.803 \]

\[ C_{T2} := 1.218 \cdot (f_1 \cdot C_b + N_{\text{trays}} \cdot f_2 \cdot f_3 \cdot C_{T1} + C_{P1}) = 428328.574 \] $\]

\[ C_{\text{Tot}} := F_M \cdot C_{T2} = 1284985.722 \] $\]

Operational Costs of the distillation column:

**Condenser:**

\[ Cooling_{\text{Cost}} := 0.03 \cdot \frac{\$}{m^3} \quad \text{Duty} := 2127472.7 \cdot 10^3 \cdot \frac{J}{\text{hr}} \]

\[ C_p := 4.187 \cdot 10^3 \cdot \frac{J}{kg \cdot K} \quad dT := 42 \text{ K} \]

\[ \text{mass} := 12097.95 \frac{kg}{hr} \quad \text{Myear} := \text{mass} \cdot 8200 \text{ hr} = 99203190 \text{ kg} \]

\[ \rho := 1000 \frac{kg}{m^3} \]

\[ V := \frac{\text{Myear}}{\rho} = 99203.19 \ m^3 \]

\[ Cost := Cooling_{\text{Cost}} \cdot V = 2976.096 \] $

**Reboiler:**

\[ Q_{\text{Duty}} := 2093389.9 \cdot 10^3 \cdot \frac{J}{\text{hr}} = 551.153 \ \text{BTU}/s \]

\[ U_o := 0.025 \ \frac{\text{BTU}}{s \cdot ft^2} \quad \Delta T := 40 \text{ F} \]

\[ A := \frac{Q_{\text{Duty}}}{U_o \cdot \Delta T} = 551.153 \ \text{F} \cdot ft^2 \]

\[ C_p := 1.95 \cdot 10^3 \cdot \frac{J}{kg \cdot F} \]

\[ Q_{\text{Duty}} = \text{mdot} \cdot C_p \cdot \Delta T \]

\[ \text{mdot} := \frac{Q_{\text{Duty}}}{C_p \cdot \Delta T} = 26838.332 \ \frac{kg}{hr} \]

\[ \$ := 1 \]
1 ton = 907.185 kg

\[ C_{\text{steam}} := \frac{\$ \cdot 6.6}{\text{ton}} = 0.007 \frac{1}{\text{kg}} \]

\[ N_{\text{hr per year}} := 8200 \frac{\text{hr}}{\text{yr}} \]

\[ C_{\text{op. reboiler}} := \text{mdot} \cdot C_{\text{steam}} \cdot N_{\text{hr per year}} = 1601096.741 \frac{\$}{\text{yr}} \]

**Total Bare Module Cost:**

\[
C_{\text{Pumps}} := 26159.80 \quad C_{\text{Reactor}} := 761648.94 \quad C_{\text{Dist_Col}} := 1284985.722 \quad C_{\text{Dev}} := 877444.517 \\
C_{\text{Agitator}} := 70638.27 \quad C_{\text{Hex}} := 101775.25 \\
C_{\text{FE}} := C_{\text{Reactor}} + C_{\text{Dist_Col}} + C_{\text{Agitator}} + C_{\text{Hex}} + C_{\text{Dev}} = 3096492.699 \\
C_{\text{PM}} := C_{\text{Pumps}} = 26159.8 \\
C_{\text{Spare}} := 0.05 \cdot C_{\text{FE}} \quad C_{\text{Storage}} := 0.02 \cdot C_{\text{FE}} \quad C_{\text{Startup}} := 0.03 \cdot C_{\text{FE}} \\
C_{\text{TBM}} := C_{\text{FE}} + C_{\text{PM}} + C_{\text{Spare}} + C_{\text{Storage}} + C_{\text{Startup}} = 3432301.769 \quad \$
\]

**Direct Permanent Investment Cost:**

\[
C_{\text{Land}} := 1136075.65 \quad \$
\]

\[
C_{\text{TBM}} = 3432301.769 \quad \$
\]

\[
C_{\text{Site}} := 0.10 \cdot C_{\text{Land}} \quad C_{\text{Serv}} := 0.20 \cdot C_{\text{TBM}} \quad C_{\text{Utility}} := 0.111 \cdot C_{\text{TBM}} = 380985.496 \quad \$
\]

\[
C_{\text{DPI}} := C_{\text{TBM}} + C_{\text{Site}} + C_{\text{Serv}} + C_{\text{Utility}} = 4613355.184 \quad \$
\]
Total Depreciable Capital:

\[ C_{DPI} = 4613355.184 \] $ \quad C_{Cont} := 0.25 \cdot C_{DPI} \quad C_{Con} := 0.03 \cdot C_{DPI} = 138400.656 \\

\[ C_{TDC} := C_{DPI} + C_{Cont} + C_{Con} = 5905094.636 \] $ \\

Total Permanent Investment:

\[ C_{TDC} = 5905094.636 \] $ \quad C_{Land} := 1136075.65 \] $ \quad C_{Royal} := 0.02 \cdot C_{TDC} \quad C_{Startup} := 0.3 \cdot C_{TDC} = 1771528.391 \\

30% for new process

\[ C_{TPI} := C_{TDC} + C_{Land} + C_{Royal} + C_{Startup} = 8930800.569 \] $ \\

Investment Site Factors:

\[ F_{ISF} := 1.0 \quad \text{Gulf Coast} \quad C_{TPI} = 8930800.569 \] $ \\

\[ C_{starTPI} := C_{TPI} \cdot F_{ISF} = 8930800.569 \] $ \\

Total Capital Investment:

\[ C_{TPI} = 8930800.569 \] $ \quad C_{WC} := 10422963.417 \] $ \\

\[ C_{TCI} := C_{TPI} + C_{WC} = 19353763.986 \] $ \quad *\text{Raw materials(1 month)} \quad *\text{Labor(52 weeks of salaries, 1 month wages)} \\

\[ C_{TCI} := C_{TCI} \cdot \frac{1}{yr} = 19353763.986 \] $ \quad *\text{Inventory of materials, products, and byproducts(1 month)} \]

Non-Commercial Use Only
Sales Revenue:

\[ P_{\text{Polymer}} := 50000 \text{ ton/yr} \]
\[ C_{\text{Polymer}} := P_{\text{Polymer}} \cdot \frac{\$}{\text{ton}} \cdot 10000000 = 10000000 \text{ \$} \]

Costs of Feedstocks:

\[ F_{\text{AIBN}} := 1649.03 \text{ ton/yr} \]
\[ F_{\text{Methanol}} := 21567.16 \text{ ton/yr} \]
\[ F_{\text{Hydroquinone}} := 0.514777 \text{ ton/yr} \]
\[ F_{\text{VAM}} := 50323.378 \text{ ton/yr} \]

\[ C_{\text{AIBN}} := F_{\text{AIBN}} \cdot \frac{$}{\text{ton}} \cdot 5443 = 8975670.29 \text{ \$} \]
\[ C_{\text{VAM}} := F_{\text{VAM}} \cdot \frac{$}{\text{ton}} \cdot 1158 = 58274471.724 \text{ \$} \]
\[ C_{\text{Methanol}} := F_{\text{Methanol}} \cdot \frac{$}{\text{ton}} \cdot 226 = 4874178.16 \text{ \$} \]
\[ C_{\text{Hydroquinone}} := F_{\text{Hydroquinone}} \cdot \frac{$}{\text{ton}} \cdot 18143.7 = 9339.959 \text{ \$} \]

\[ C_{\text{Feedstocks}} := C_{\text{AIBN}} + C_{\text{VAM}} + C_{\text{Methanol}} + C_{\text{Hydroquinone}} = 72133660.133 \text{ \$} \]

Cost of Utilities:

Cooling and Heating Utilities:

\[ \Sigma_{\text{Cooling_Utilities}} := 271580 \text{ m}^3/\text{yr} \cdot \frac{$}{\text{m}^3} \cdot 0.03 = 8147.4 \text{ \$} \]
\[ \Sigma_{\text{Steam_Utilities}} := 242590.33 \text{ ton/yr} \cdot 6.6 \text{ \$} = 1601096.178 \text{ \$} \]
\[ \Sigma_{Heating\_Utilities} := 57572.70 \frac{m^3}{yr} \cdot \frac{\$}{m^3} = 2878.635 \frac{\$}{yr} \]

\[ \Sigma_{Electricity} := 102.84 \frac{kW \cdot hr}{yr} \cdot \frac{\$}{kW \cdot hr} = 54139.09 \frac{\$}{yr} \]

\[ \Sigma_{Waste} := 0.33 \frac{\$}{kg} \cdot 72.412 \frac{kg}{hr} \cdot 8200 \frac{hr}{yr} = 195946.872 \frac{\$}{yr} \]

\[ C_{Util} := \Sigma_{Electricity} + \Sigma_{Heating\_Utilities} + \Sigma_{Cooling\_Utilities} + \Sigma_{Waste} + \Sigma_{Steam\_Utilities} = 1862208.175 \frac{\$}{yr} \]

\[ C_{F\&U} := C_{Util} + C_{Feedstocks} = 73995868.308 \frac{\$}{yr} \]

**Cost of Manufacturing:**

**Labor-related Operational Costs:**

\[ \text{workhours} = 40 \frac{hr}{week} \cdot 52 \text{ weeks} = 2080 \text{ hrs} \quad \text{workhours} := 2080 \frac{hr}{yr} \]

\[ C_{Oper} := \frac{\$}{hr} \cdot 50 = 8200 \frac{hr}{yr} = 3.942 \]

\[ N_{Ops} = \frac{24 \text{ Operators}}{4 \text{ Shifts}} = 6 \frac{\text{Operators}}{\text{Shift}} \quad N_{Ops} := 6 \]

\[ DW\&B := C_{Oper} \cdot N_{Ops} \cdot N_{Shifts} \cdot \text{workhours} = 2460000 \frac{\$}{yr} \]

\[ SDW\&B := 0.15 \cdot DW\&B = 369000 \frac{\$}{yr} \quad N := 1 \]

\[ TechAssist := \frac{\$}{yr} \cdot 60000 = 60000 \frac{\$}{yr} \quad N := 2 \]

\[ Control\_Lab := \frac{\$}{yr} \cdot 60000 \cdot N = 120000 \frac{\$}{yr} \]
\[ C_{Op} := 1.21 \cdot DW\&B + TechAssist + Control\_Lab = 3156600 \text{ $/yr} \]

**Cost of Maintenance:**

\[ C_{TDC} = 5905094.636 \text{ $/yr} \quad MW\&B := \frac{0.045}{\text{yr}} \cdot C_{TDC} = 265729.259 \text{ $/yr} \]

\[ C_{TDC} := C_{TDC} \cdot \frac{1}{\text{yr}} = 5905094.636 \text{ $/yr} \]

\[ C_{Maint} := 2.3 \cdot MW\&B = 611177.295 \text{ $/yr} \]

\[ SMW\&B := 0.25 \cdot MW\&B = 66432.315 \text{ $/yr} \quad MW\&B = 265729.259 \text{ $/yr} \]

**Cost of Manufacturing: Operating Overhead**

\[ M\&O\_SW\&B := DW\&B + SDW\&B + MW\&B + SMW\&B = 3161161.573 \text{ $/yr} \]

\[ Gen\_Plant\_Overhead := 0.071 \cdot M\&O\_SW\&B = 224442.472 \text{ $/yr} \]

\[ Mech\_Dept := 0.024 \cdot M\&O\_SW\&B = 75867.878 \text{ $/yr} \]

\[ Emp\_Rel\_Dept := 0.024 \cdot M\&O\_SW\&B = 75867.878 \text{ $/yr} \]

\[ Bus\_Services := 0.074 \cdot M\&O\_SW\&B = 233925.956 \text{ $/yr} \]

\[ C_{Ov} := 0.193 \cdot M\&O\_SW\&B = 610104.184 \text{ $/yr} \]

**Cost of Operations: Taxes, Insurance, and Depreciation**

\[ C_{TDC} = 5905094.636 \text{ $/yr} \quad C_{alloc} := C_{Utility} = 380985.496 \text{ $} \]

\[ C_{Tei} := 0.02 \cdot C_{TDC} = 118101.893 \text{ $/yr} \]

\[ C_{TDC} = 5905094.636 \text{ $/yr} \quad C_{alloc} = 380985.496 \]
\[ C_{TDC} := C_{TDC} \cdot \text{yr} = 5905094.636 \ $ \]

\[ D_{PO} := \frac{0.08}{\text{yr}} \cdot (C_{TDC} - 1.18 \cdot C_{alloc}) = 436442.54 \ \frac{\$/\text{yr}}{} \]

\[ D_{AP} := \frac{0.06}{\text{yr}} \cdot 1.18 \cdot C_{alloc} = 26973.773 \ \frac{\$/\text{yr}}{} \]

\[ C_{Dep} := D_{PO} + D_{AP} = 463416.313 \ \frac{\$/\text{yr}}{} \]

**COM: Cost of Manufacture**

\[ C_{Feedstocks} = 72133660.133 \ \frac{\$/\text{yr}}{} \]

\[ C_{Util} = 1862208.175 \ \frac{\$/\text{yr}}{} \]

\[ C_{Op} = 3156600 \ \frac{\$/\text{yr}}{} \]

\[ C_{Maint} = 611177.295 \ \frac{\$/\text{yr}}{} \]

\[ C_{Ov} = 610104.184 \ \frac{\$/\text{yr}}{} \]

\[ C_{T&I} = 118101.893 \ \frac{\$/\text{yr}}{} \]

\[ C_{Dep} = 463416.313 \ \frac{\$/\text{yr}}{} \]

\[ COM := C_{Feedstocks} + C_{Util} + C_{Op} + C_{Maint} + C_{Ov} + C_{T&I} + C_{Dep} = 78955267.992 \ \frac{\$/\text{yr}}{} \]

**Costs: General Expenses**

\[ COM = 78955267.992 \ \frac{\$/\text{yr}}{} \]

\[ GE := 0.1 \cdot COM = 7895526.799 \ \frac{\$/\text{yr}}{} \]

\[ C := COM + GE = 86850794.792 \ \frac{\$/\text{yr}}{} \]

**Working Capital**

\[ CR := \left( \frac{COM}{12} \right) = 6579605.666 \ \frac{\$/\text{yr}}{} \]

\[ Inv := 1521162.76 \ \frac{\$/\text{yr}}{} \]
\[ AcctPay := \frac{C_{Feedstocks}}{12} = 6011138.344 \ $ \text{ yr} \]
\[ AcctRec := \frac{C_{Polymer}}{12} = 8333333.333 \ $ \text{ yr} \]

\[ C_{WC} := CR + Inv + AcctRec - AcctPay = 10422963.415 \ $ \text{ yr} \]

**Gross and After Tax Earnings**

\[ S := 50000 \ \frac{ton}{yr} \cdot \frac{\$ \cdot 2000}{ton} = 100000000 \ $ \text{ yr} \]

\[ C := COM + GE = 86850794.792 \ $ \text{ yr} \]

\[ GPT := S - C = 13149205.208 \ $ \text{ yr} \]

\[ NPT := 0.63 \cdot GPT = 8283999.281 \ $ \text{ yr} \]

**Profitability:**

\[ ROI := \frac{NPT}{C_{TCI}} = 0.428 \]

\[ i_m = 0.025 \quad C_{TCI} = 19353763.986 \ $ \text{ yr} \]

\[ C_{TDC} = 5905094.636 \ $ \]

\[ PBP := \frac{C_{TDC}}{NPT + C_{Dep}} = 0.675 \text{ yr} \]

\[ VP := NPT - i_m \cdot C_{TCI} = 7800155.182 \ $ \text{ yr} \]

Risk Assessment: 25% High