The Production of Cyano Dyes

Annual Plant Capacity of 50,000 kg

Final Report

Deliverable Date: Monday, November 19, 2018

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Team Number: 15
Team Members: Anita Ankisetty
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Wallberg Chemical Production Inc.

Table of Contents

Executive Summary

Our engineering firm, Wallberg Chemical Production Inc., was hired by Dr. Marko Saban to deliver a Process Design Basis report for the production of 50,000 kg/year of alkylphenoxy-metallic phthalocyanines (hereby referred to as alkylphenoxy-MPcs). Alkylphenoxy-MPcs are organic ligands that can be designed as waxy, highly pigmented, blue or cyan dyes. As the world's second most important class of colourant, these dyes have high industrial value. Currently, Xerox owns the patent outlining the production of alkylphenoxy-MPcs, and holds a monopoly over market shares and prices. Our client plans to market this product as a lower-cost alternative for inkjet printing purposes.

Production of alkylphenoxy-MPcs involves a two-step reaction and purification, as dictated by US Patent 6,476,219. Our team evaluated the 14 examples included in the patent to determine which process best suits our objectives. The team chose to scale up patent examples 4 and 8. Example 4 outlines the SNAr reaction of 3-pentadecylphenol and 4-nitrophthalonitrile to produce the intermediate MPc adduct, and example 8 details the formation of the final alkylphenoxy-MPc.

Based on these patent examples, the team developed two Process Flow Diagrams. From this, an equipment list was developed, highlighting the jacketed batch reactor and 2 Nutsche filters as integral to the design. This led to us to select the 1900 US gallon batch reactor as our key design unit. Further design and analysis was performed, including identification of operating conditions, control systems, and startup/shutdown procedures.

Moving forward, the site-wide layout and plant schematic were developed to identify the placement of required facilities and account for safe distance planning between operations and major equipment.

Our team considered possible safety concerns, environmental constraints, and legal requirements, incorporating solutions to mitigate risks and reduce operating costs. Furthermore, an economic analysis was conducted to determine the feasibility of this project, resulting in a recommended price per kg to sell the final product.

Upon submission of this report, Wallberg Chemical Production Inc. recommends that the client perform further laboratory analysis of the selected patented examples to optimize the process, reducing both overall cycle time to produce the final product and operating costs (i.e. raw material costs, waste disposal costs).

Wallberg Chemical Production Inc.

Attribution Table

Table 1: Summary of the team members' main contributions to the design project

Team Member	Chief Responsibility	Deputy Responsibility
Nyat Habtit	Plant Layout Equipment List Environmental Assessment	Safety Analysis Tank Sizing
Anita Ankisetty	Block Flow Diagram Mass Balance Key Unit P&ID	Equipment List Process Flow Diagrams
Jeffrey Dryden	Process Flow Diagrams Energy Balance 3D SketchUp Model	Mass Balance Key Unit P&ID
Claude Nnadi	Tank Sizing Safety Analysis Legal Requirements/Considerations	3D SketchUp Model Plant Layout Economics
Henry Wu	Economic Analysis Raw Materials Sourcing	Block Flow Diagrams Mass Balance

Name: Nyat Habtit

Signature: 

Name: Anita Ankisetty

Signature: 

Name: Jeffrey Dryden

Signature: 

Name: Claude Nnadi

Signature: 

Name: Henry Wu

Signature: 

1.0 Scope of Design

1.1 Project Charter

The project charter outlines the scope, requirements, and participants in the design project, providing a brief summary of the expected project outcome.

Table 2: Project charter for the production of cyano dyes design project

<table>
<tr><td>Project Name</td><td colspan="5">The Production of Cyano Dyes</td></tr>
<tr><td>Project Description</td><td colspan="5">The client has requested the design of a complete process to produce alkylphenoxy-phthalocyanines in a blue or cyan hue for solid ink printing.</td></tr>
<tr><td colspan="3">Project Goal</td><td colspan="3">Business Case</td></tr>
<tr><td colspan="3">Prepare a Process Design Basis report for the production of 50,000 kg/year of alkylphenoxy-phthalocyanines.</td><td colspan="3">As a chemically stable dye used in various industry applications, this product is economically valuable.</td></tr>
<tr><td colspan="3">Scope</td><td colspan="3">Worked Hours</td></tr>
<tr><td colspan="3">The scope of this design project will include raw materials sourcing, process design, special design of a key unit, 3D simulation, process safety review, environmental assessment, and economic analysis.</td><td colspan="3">The team budgeted a total of 720 hours for completion of this project. Upon submission, 610 engineering hours were billed as part of the project expenses.</td></tr>
<tr><td colspan="3" rowspan="5">Participating Organizations

Engineering Firm: Wallberg Chemical Production Inc.

Client: Dr. Marko Saban

Project Sponsor: Dr. Timothy Bender

Patent Holder: Xerox</td><td>Deliverables</td><td>Deadlines</td></tr>
<tr><td>1. Proposal</td><td>Sept. 20, 2018</td></tr>
<tr><td>2. PFD</td><td>Oct. 5, 2018</td></tr>
<tr><td>3. Key Unit P&ID</td><td>Oct. 22, 2018</td></tr>
<tr><td>4. Final Report</td><td>Nov. 19, 2018</td></tr>
<tr><td colspan="5">Team Members</td><td>5. Presentation</td><td>Nov. 27, 2018</td></tr>
<tr><td>Nyat Habtit,
Team Leader</td><td>Anita Ankisetty,
Deputy Leader</td><td>Jeffrey Dryden,
Team Member</td><td>Claude Nnadi,
Team Member</td><td colspan="2">Henry Wu,
Team Member</td></tr>
</table>





1.2 Gantt Chart

The Gantt chart illustrates the planned and actual project schedule (refer to Appendix A). During the course of the project, it was maintained and updated to track the team's progress. Initially, the team had overestimated the amount of time required to complete certain deliverables, such as economic analysis of our plant. Moreover, other tasks required several revisions, extending some internal deadlines. As the design process continued, the Gantt chart was closely monitored to ensure that any deliverables and check-in dates were met.

Overall, the team allotted approximately 720 engineering hours for completion of this project (refer to Appendix B). Task completion was tracked using the Gantt chart and hours worked were tracked with a time log. Subsequently, the team was able to estimate and validate the engineering expenses towards the project budget. Having contributed 610 total hours to this project and assuming an average engineering salary in Canada to be $31.00/hour [1] with a 20% profit margin, the total engineering cost of this project is $22,692 CAD.

1.3 Chemistry Background

Metallic phthalocyanines (hereby referred to as MPcs) are aromatic, macrocyclic organic compounds, bonded with a central metal atom. Copper phthalocyanines are the most important metallic derivative due to their bright colour and high structural resonance stability [2]. Generic MPcs are insoluble pigments, and must become functionalized for use in industry applications [2]. Alkylphenoxy-MPcs, as seen in figure 1, are a soluble alternative that can be used in a variety of applications due to its high, generic solubility [3].

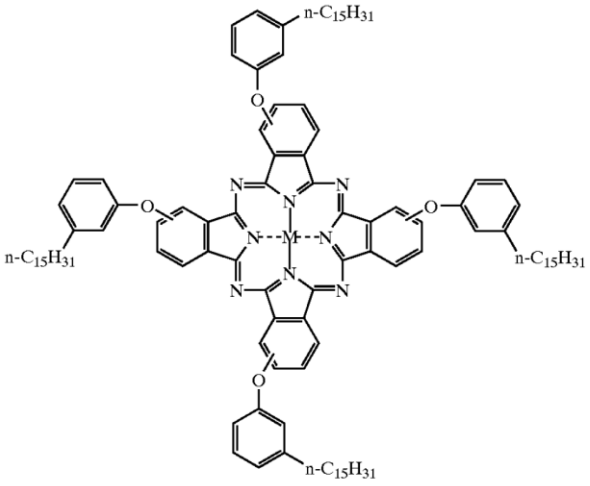

Figure 1: Chemical composition of alkylphenoxy-MPc [2]

The current industry process for MPc synthesis makes use of a two-step process, as dictated by the US Patent 6,476,219 [2]. First, 3-n-pentadecylphenol (hereby referred to as 3PDP) is reacted with 4-nitrophthalonitrile (hereby referred to as 4NPN) in the presence of a base and heat to form an intermediate, the MPc adduct (refer to Appendix C) [2]. The resulting adduct is added to a metal compound, or ammonia-releasing compound, to form the final MPc colorant (refer to Appendix D) [2].

1.4 Problem Statement

MPcs are man-made colourants that are widely used in making pigments for automotive paints, printing inks, and dyes [2]. As the world's second most important class of colourant, they possess a high commercial value and a range of useful properties. They are used in high technology applications such as inkjet printing, charge generation materials for laser printers, light sensors in photovoltaic solar cells and photosensitizers for cancer therapy [2]. On the visible spectrum, MPcs are limited to three colours: cyan, blue, and green [2]. However, they can be chemically engineered to absorb infrared rays for other high technology applications [2].

Our company, Wallberg Chemical Production Inc., has been contracted by Dr. Marko Saban to develop a complete process for the production of alkylphenoxy-MPcs. He intends to develop an industrial scale plant to produce these MPcs to be used in eco-friendly solid ink printing dyes. The production of these MPcs will require a two-step synthesis process and purification, as described in US Patent 6,476,219 [2]. Currently, Xerox holds ownership of this patent and is the sole producer of these MPcs for the purposes of solid ink printing. As the current market needs are met by a toll vendor, they have a monopoly on the price of the dye; as the market shifts away from inkjet printing towards electronic media, and market volume decreases, the vendor can increase the price. Upon expiry of the Xerox patent, there will be an opportunity to introduce a lower-cost alternative MPc to the market.

Furthermore, the client has expressed his passion for sustainable manufacturing and green chemistry. As emerging experts in this field, our team plans to make use of the 12 principles of green chemistry, as outlined by the American Chemical Society, to align the process with our client's priorities [4]. For instance, one of the key chemicals in producing MPcs, 3PDP, is sourced from a derivative of cashew nut shell liquid (hereby referred to as CNSL) [5]. CNSL is considered a renewable feedstock material, minimizing the impact of the process on the local environment and contributing to a sustainable business model.

1.5 Scope

Wallberg Chemical Production Inc. is providing a comprehensive report, inclusive of front-end loading stages 1 through 3.

The following elements are out of scope of this design and are excluded from this report:

- Formulation of the MPc product into solid inkjet printing materials
- Transportation of the MPc product outside of the manufacturing site

- Stages of the design process outside FEL-1, FEL-2 and FEL-3 (i.e. EPC)

Our team has identified the requirements, objectives, and constraints for this project.

1.5.1 Requirements

- The plant must have a minimum annual capacity of 50,000 kg/year
- The MPc must have a blue or cyan hue
- The MPc must be waxy and soluble in the ink matrix

1.5.2 Objectives

- The patent processes should be evaluated and selected for scale-up
- The final product should have a minimum product purity of 98%
- The yield of the first step of the process should be 80% to 90%
- The yield of the second step in the process should be above 70%
- The process design should incorporate sustainable manufacturing principles
- The plant should have a minimum payback of five years

1.5.3 Constraints

- The plant will be located in the chemical sector of Sarnia, Ontario (refer to Appendix E)
- All designs and operations must be in compliance with federal/provincial regulations and municipal bylaws, such as O. Reg. 169/03, 675/98 and 381/15 (see section 9.0 for more details)

1.6 Proposed Solution

The engineering team is presenting the client with the following proposed solution that meets the project requirements.

1.6.1 Patent Processes

US Patent 6,476,219 was used to select the process for production of the MPc final product. The patent contains 14 different examples, which either produced the MPc adduct, the MPc final product, or produced the final product in a one-step reaction. Furthermore, not every example provided in the patent produced the same product. Several examples used tin and zinc as the metallic centres of the MPc, and two examples produced a non-metallic MPc.

The processes described in the patent examples were all performed on a laboratory scale. Upon evaluation of the patent examples, the selected examples were scaled up to meet the required plant production target.

1.6.2 Evaluation of Patent Examples

The patent examples were evaluated against the team's priorities. The following is a list of weighted priorities identified by the team, through discussions with the client:

1. Personnel safety (i.e. occupational health & toxicity)
2. Environmental & chemical safety
3. Economics (i.e. preliminary raw materials costs)
4. Product purity
5. Product yield
6. Product volume
7. Space (of the process equipment within the plant)
8. Personnel efficiency (i.e.operators required, maintenance, and process upkeep)

The top five priorities were used to create a priority matrix to evaluate the patent examples (refer to Appendix G). Decision making matrices were then used to evaluate patent examples 1 to 10. Examples 11 to 14 were removed from the scope of this evaluation as they did not meet the objectives of the design.

With regards to the first two criteria (toxicity, safety) the solvent used in each example was evaluated based on the Sanofi Solvent Selection Guide [6]. This was the focus of the safety evaluation, as large quantities of the solvent would be used in the process, thus providing the greatest risk. The economics were evaluated based on the preliminary raw material costs (RMC) for each example (refer to Appendix F). The remaining criteria (purity, yield) were evaluated based on the information provided by the patent.

1.6.3 Chemistry Process Considerations

When developing the process, our team considered optimizing the selected patent processes to reduce costs, increase efficiency, and follow sustainable practices. Furthermore, our team wanted to retain in-house expertise, rather than outsource key elements of our process. In doing so, the client would have more control over the profitability of this project and would not be subject to any contractors' demands or prices.

To do this, our team considered in-house production of 3PDP through the hydrogenation of cardanol, rather than purchasing it from a supplier. In each batch process producing the MPc adduct, 3PDP accounts for approximately 20% of the reaction mixture making it a key reagent in our process.

If producing it internally is reasonably safe, economically feasible, and does not impose new hazards into the plant, it may prove to be a viable solution.

Cardanol,a derivative of CNSL, is considered a sustainable source of the 3PDP raw material [5]. Through three phase catalytic hydrogenation in a slurry reactor, the cardanol is reacted as follows:

$$C_6H_4OHC_{15}H_{25} + 3H_2 \rightarrow C_6H_4OHC_{15}H_{31} \qquad \Delta H° = -359.87 \text{ kJ/mol [7]}$$

Upon consideration of the safety, toxicity, and economic feasibility (refer to Appendix G), the team decided against the internal production of 3PDP. The hydrogenation of cardanol is relatively more expensive than purchasing 3PDP, and the hydrogenation process requires large amount of hydrogen gas,

imposing a serious safety concern. Thus, 3PDP will be purchased and acceptable costs can be negotiated with the supplier.

1.6.4 Selected Patent Examples

Patent examples 4 and 8 were chosen based on the results of the decision making matrices (refer to Appendix G).

Example 4 was chosen for the first step of the process, which produces the MPc adduct. This patent example was selected based on the toxicity of the solvent (DMSO), RMC, high product purity, and high yield.

Example 8 was chosen for the second step of the process, which produces the MPc final product. This patent example was selected for its competitive RMC, high product purity, and high yield. However, example 8 uses NMP as a solvent, which is reprotoxic and can impose adverse health effects. As there were no other acceptable alternatives identified for this step of the process, our team will carefully consider the toxicity and safety of NMP throughout the design.

The procedure for example 4 is as follows:

"To a 5 liter 1-necked round bottomed flask equipped with mechanical stirrer was added 502.5 grams (1.65 mole) of 3-pentadecylphenol, 200 grams (1.45 mole) of 4-nitrophthalonitrile, and 2,000 grams of dimethylsulfoxide (DMSO). The mixture was heated to 90ºC. for 3 hours using a heating mantle. The reaction mixture turned dark brown. The reaction mixture was then cooled to 80ºC., and was quenched by slowly pouring 3 liters of deionized water into the flask. The precipitated beige solid was stirred until the suspension had cooled to room temperature, then was separated by filtration. It was then twice slurried and filtered using about 6 liter portions of deionized water. The wet cake was then stirred for 1 hour in 6 liters of 2 percent aqueous hydro chloric acid, which served to dissolve small amounts of insoluble metal carbonate contaminants, then was filtered. It was slurried, filtered, and reslurried in 6 liter potions of deionized water until the water used to wash the solid product was of neutral pH. The solids were then twice slurried in 4 liters of methanol, filtered, and vacuum dried at 40ºC. to give 558.4 grams (90 percent yield) of 4-(3-pentadecyl) phenoxyphthalonitrile. The purity of this material as measured by HPLC was over 98 percent." [2]

The procedure for example 8 is as follows:

*"A solution of 60.8 grams (0.14 mole) of 4-(3-pentadecyl) phenoxyphthalonitrile in 195 milliliters of NMP in a 500 milliliter flask fitted with a mechanical stirrer, maintained under a nitrogen atmosphere, was treated with 6.24 grams (0.031 mole) of copper (II) acetate monohydrate, and 6.24 grams (0.070 mole) of 2-dimethylaminoethanol (DMAE). The mixture was stirred and heated at 180ºC. for 6 hours, then was cooled to 80ºC. The mixture was then filtered, and the solid was washed in the filter with 120 milliliters of NMP. The solid was then slurry-washed and filtered three times with 120 milliliter portions of methyl ethyl ketone. Drying for 48 hours at 30ºC. under vacuum gave the product as a coarse blue powder (44 grams, 80 percent). The spectral strength of this dye was 1.28x10^5 A*mL/g, indicating a purity of over 98 percent."* [2]

2.0 Process Evaluation

The selected patent examples were analyzed to create block flow diagrams, and develop the mass and energy balance for the process.

2.1 Block Flow Diagram

Block flow diagrams (BFD) were developed to scale up the laboratory process for each step. The BFD for step 1, the production of the MPc adduct, is based on patent example 4. The scaled up mass balance is included in the BFD (refer to Appendix H).

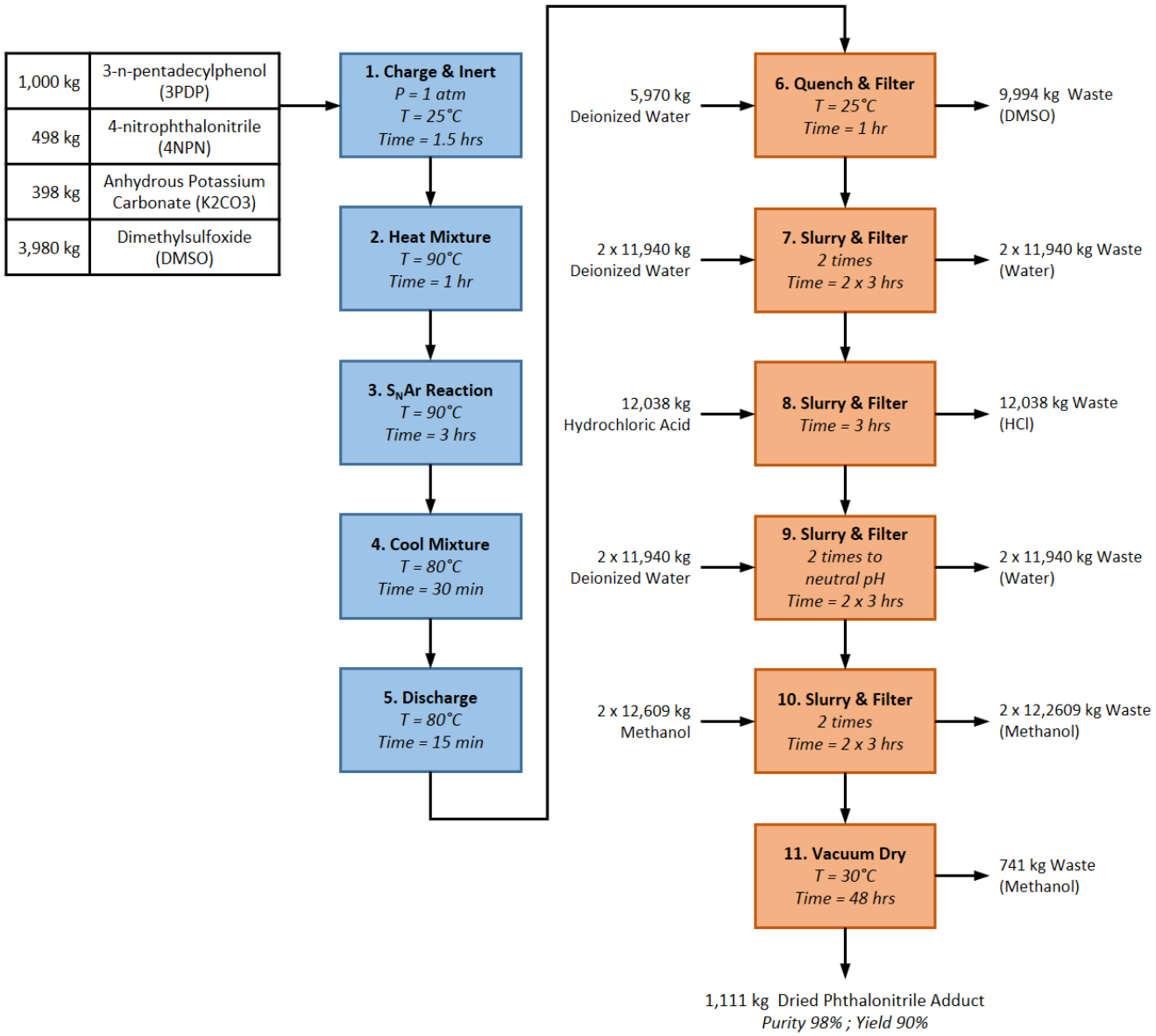

Figure 2: Block Flow Diagram for step 1, based on patent example 4.

The BFD for step 2, the production of the final product, is based on patent example 8. The scaled up mass balance is included in the BFD (refer to Appendix H, table 11).

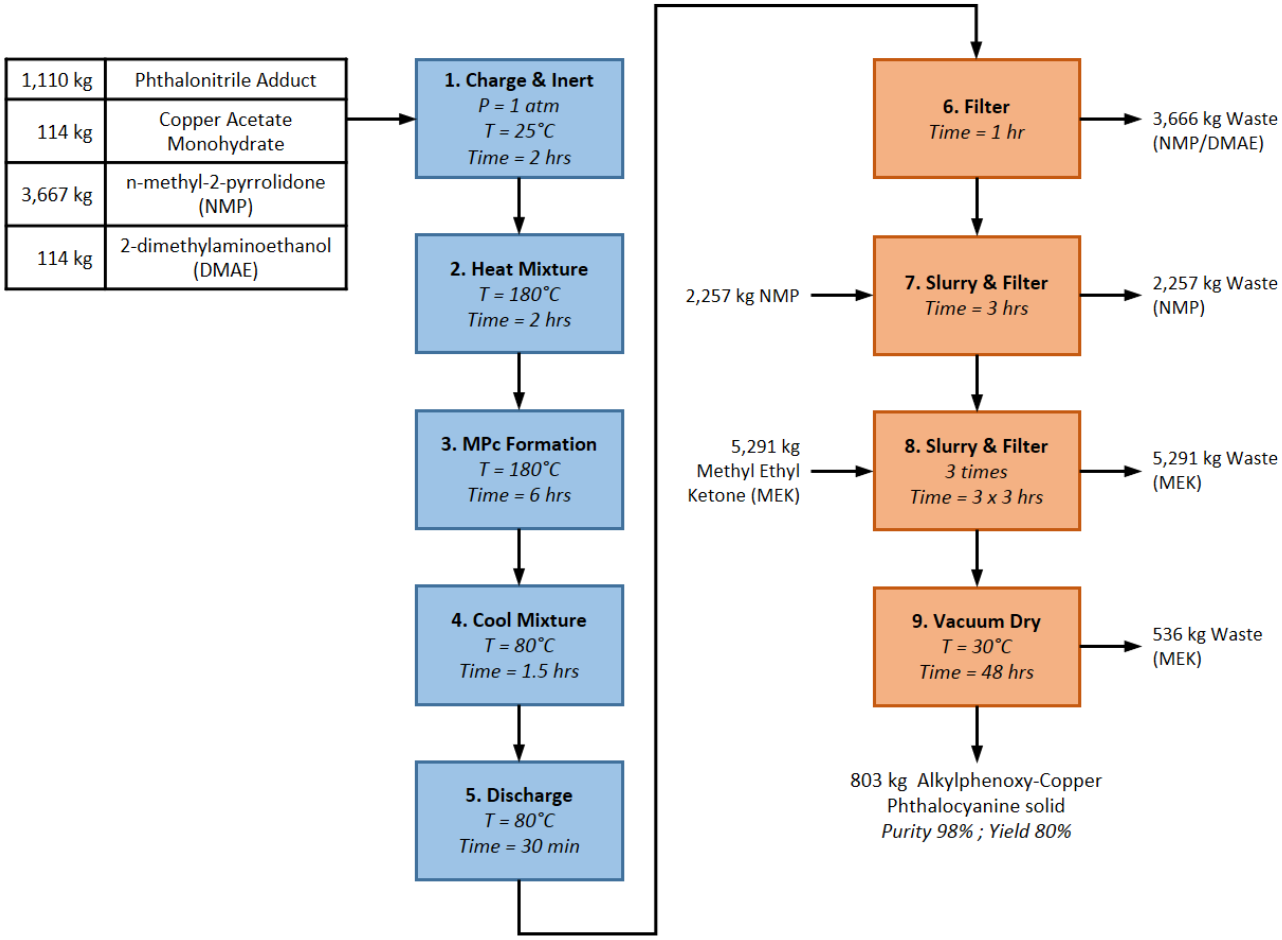

Figure 3: Block Flow Diagram for step 2, based on patent example 8

Using the BFD, the team identified two crucial pieces of equipment for this process - a jacketed batch reactor and a filter. The blue blocks indicate stages of the reaction that will be performed in the reactor, and the orange blocks indicate stages of the reaction that will occur in the filter. Selection and further design of this equipment is discussed in sections 3.0 and 4.0.

2.2 Mass Balance

The BFD above includes an overall mass balance for the process (refer to Appendix H). To determine the mass of reactants/solvents required for each batch, a scale-up factor was applied to the patent example. The scale up factor was developed based on the cycle time of each step, the plant up-time, production schedule, and the target production rate of 50,000 kg/yr (refer to Appendix I). The outcome of the mass balance is that step 1 will produce 1,111 kg of MPc adduct per batch, and step 2 will produce 803 kg of MPc final product per batch.

Each process uses a series of slurries to purify the MPc adduct and final product. Within the mass balance, it was assumed that after each filtration step, a wet cake remains which is composed of 60% solid product and 40% washing solvent, by mass. This accounts for the liquid that remains after a solid has been filtered. At the end of each step, this wet cake is vacuum dried to remove all remaining liquid and yields a dry, solid product.

2.3 Energy Balance

The energy balance was calculated around both steps of this process (refer to Appendix K). First, the time required to heat the reactor using the heating jacket was calculated. This is combined with the reactor charging time to make up the start-up time for each reaction. During step 1 of the reaction, the mixture is heated from 25ºC to 90ºC. During step 2, the mixture is heated from 25ºC to 180ºC. Since step 2 of the reaction is heated to double the temperature of step 1, the heating time is approximately 50% longer. To account for any thermal losses and extra time required to heat the mixture in an industry setting, an additional scale-up factor of 30% was applied to the calculated heating times. The time required to heat step 1 is 0.94 hours (3,353 seconds), and the time required to heat step 2 is 1.3 hours (4,696 seconds).

Maintaining the reaction temperature of the reacting mixture is determined based on the following assumption. While the exact thermodynamics of the reaction are unknown, the reaction is assumed to be mildly exothermic due to the large quantity of solvent that will be present. Therefore, it is assumed that any heat gained from the reaction is equal to the heat lost to the reactor's surroundings.

The time required to cool the reaction mixture following the reaction was calculated (refer to Appendix K). During step 1 of the reaction, the mixture is cooled from 90ºC to 80ºC before being moved to the filter. During step 2, the mixture is cooled from 180ºC to 80ºC. The time to cool was calculated and the scale-up factor of 30% was applied. The time required to cool step 1 is 0.25 hours (879 seconds), and the time required to cool step 2 is 1.05 hours (3,784 seconds).

Finally, the reactor reflux condenser was sized (refer to Appendix J). While not designed for heavy usage during the formation of the MPc, the condenser will be used when cleaning the batch reactor. This will involve the reflux of toluene inside the reactor, and thus the reactor jacket alone cannot be relied on to condense the toluene vapours

3.0 Overall Process

The selected patented examples were scaled up from a laboratory scale experiment. When dealing with the larger scale, three process elements were identified:

- The bulk handling of the chemicals
- The physical reaction of the chemicals
- The filtering and drying of the crude product

Our proposed solution is designed around these three process elements, to ensuring feasibility on a manufacturing plant scale.

3.1 Key Process Parameters

The onsite bulk chemical handling falls into two categories: liquids and solids handling. All liquids are transported to the plant and into the reactor via pumps and pipes (refer to Appendices M and N). In addition to the liquid chemical reagents, 3PDP is received as a waxy solid in a 200 lb drum, making it difficult to extract efficiently and safely. To use the 3PDP in our process, a drum jacket will be placed on the drum to melt the solid (at 50-53°C). Once the 3PDP is in its liquid form, it can be easily pumped into the jacketed batch reactor.

However, handling of other solids is slightly more complex. In our plant, there is a designated solid chemical dispensing area adjacent to the shipping and receiving docks for operators to safely load and unload chemicals from incoming transport trucks (refer to Appendix U). The solid chemicals will either supplied in 50 lb (22 kg) bags, like the copper (II) acetate monohydrate and anhydrous potassium carbonate, or in 200 lb (91 kg) drums, like the 4NPN. Bags of solids will be emptied into the dispensing station manually, and drums with solids will be deposited into the respective hoppers using a crane (refer to Appendix V). From the hopper, a batch weighted scale will be used to measure the weight of solids to be added [8]. Load cells will transmit signals to control the flowrate of fine solid particles by adjusting the valves' position. Figure 4 below illustrates the chemical dispensing area and batch weighted scale.

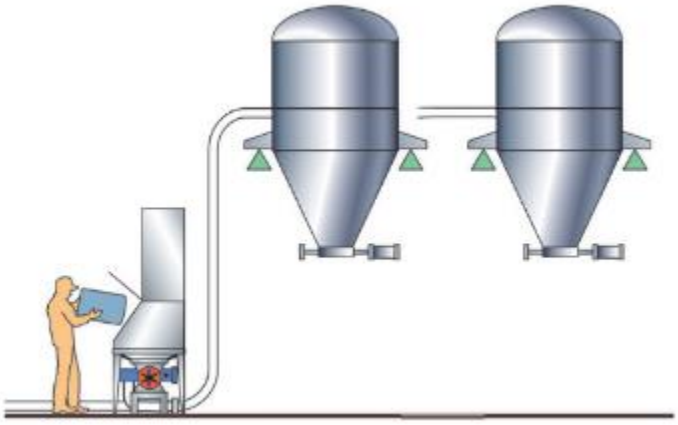

Figure 4: Bulk solids handling process [8]

When deciding on a unit to house the chemical reaction of the process, the scale of the reaction was considered. Our team decided to use a single batch reactor for this process because the scale of the reactor was considerably smaller than the scale of the filter. Using a batch reactor allows for the best mixing possible, and allows the conditions of the reaction to be properly controlled.

To purify the crude product, the process can be broken down into four parts: the charging of a liquid solvent, the slurrying and mixing of the crude product, the filtering of the slurry, and the vacuum drying. Through extensive research, our team decided to make use of a Nutsche filter-drying system, which is able to complete the four step filter process in a single, contained vessel [9]. This ensures that operators will not be exposed to any harmful chemicals or fumes, and allows for increased automation in our process.

3.2 Process Flow Diagram

As a part of the basis of design, a Process Flow Diagram (PFD) has been developed for the two-step reaction and purification process (refer to Appendices M and N). The PFD for steps 1 and 2 are very similar, as most of the equipment is used in both reactions. However, the reactants and solvents that are charged into the reactor differ between steps 1 and 2. As described in section 3.1, and depicted in the PFD, the following pieces of equipment are essential in the process:

- Batch weighing system for the bulk solids handling and measuring
- Jacketed batch reactor for the reaction of chemicals reagents
- Nutsche filters for purification of the product (2 filters to be run in parallel)

3.3 Cycle Time

During the design of our process, the cycle times and plant schedule were determined. As the cycle times were developed, we found that the times spent washing, filtering and drying the product were longest, and therefore, these were the rate limiting steps of the process. As each step requires 48 hours of vacuum drying and numerous slurries, the majority of the time spent within each cycle will be in the Nutsche filter. In order to reduce the cycle times, we decided to run two Nutsche filters in parallel, so that two batches of the same step can be run simultaneously. For both steps 1 and 2, this decision effectively reduces the average cycle time from 78 hours to 42.5-43 hours (refer to calculations in Appendix L). This provides two advantages, the first being that a single cycle can comfortably fit within a two-day period, leaving ample time for reactor maintenance if needed. Furthermore, production can alternate between processes without impacting the plant schedule, as both steps 1 and 2 have similar cycle times.

Table 3: Each stage from the patented process with scaled-up time frames

Process	Time Required for Step 1	Time Required for Step 2
Charge	2 hours	2 hours
Heat	1 hour	2 hours
React	3 hours	6 hours
Cool	30 minutes	1.5 hours
Drain	30 minutes	30 minutes
Quench	1 hour	N/A
Filter	N/A	1 hour
Slurry & Filter	21 hours (3 h x 7 slurries)	12 hours (3 h x 4 slurries)
Vacuum Dry	48 hours	48 hours

It was decided to use a campaigned production schedule to increase efficiency, reduce unnecessary cleaning between batches, and minimize the size of reagent storage tanks. Using a 42 week per year

production time frame, this allows for 21 weeks to produce the adduct using step 1 of the reaction, and 21 weeks to produce the final product using step 2. To maintain a moderate product inventory and provide customers with timely product deliveries, the decision was made to run each step for 7 weeks at a time, then switch to the next step. There will be a down-time of one week after each 7 week cycle for cleaning and maintenance of equipment. Therefore, the plant will produce and deliver the final product every 3.5 months.

In addition to the campaign schedule, our team also identified a chemical delivery schedule, which dictates the frequency of how often reagent and solvent tanks will be refilled. By performing a sensitivity analysis around the sizes of our chemical storage tanks, we found the optimal delivery frequency to be once per week (refer to Appendix L).

3.4 Material Selection

Material selection was considered for each major piece of equipment (refer to Appendix O). For most chemical processes, austenitic stainless steel is preferred over alternative stainless steels, such as ferritic, martensitic, and duplex [10]. Austenitic stainless steel is chosen for it's overall tough material properties, weldability, and general corrosion resistance [10]. One major weakness of austenitic stainless steels is a large vulnerability towards chloride stress corrosion cracking (SCC), so minimizing contact with chlorides is imperative [10].

When comparing austenitic stainless steels, there are two widely utilized grades: 304 and 316. The largest difference between the two is the inclusion of molybdenum in 316 grade stainless steel [11]. Molybdenum improves the materials corrosion resistance towards chlorides [11]. For this reason, the primary material selected for the batch reactor and the majority of storage tanks is stainless steel grade 316 (S.S. 316). Stainless steel 316 is composed of 16% chromium, 10% nickel, and 2% molybdenum [11].

While S.S. 316 is the ideal material for the batch reactor and the most storage tanks, hydrochloric acid is used as a washing solvent for the Nutsche filter in step 2 of the process. As a strong chloric acid, this would introduce rapid SCC into the unit, and is therefore not compatible with S.S. 316. Therefore, a glass-lined S.S. 316 Nutsche filter will be used, which drastically improves corrosion resistance and will reduce the overall maintenance required on the filter.

Hydrochloric acid will be stored in the tank farm at a concentration of 37%. At this high concentration, a specialty material is required to prevent corrosion. The recommended vessel to store hydrochloric acid at this concentration is a corrosion resistant polypropylene tank (refer to Appendix W).

Table 4: Summary of material selection for major pieces of equipment

Piece of Equipment	Material Choice
Batch Reactor	Stainless Steel 316
Nutsche Filter	Glass-lined Stainless Steel 316

All Tanks (Exception Hydrochloric Acid)	Stainless Steel 316
Hydrochloric Acid Tank	Corrosion Resistant Polypropylene

3.5 Equipment List

A full equipment list was developed for all major equipment in the plant, outlining the equipment type, description, electrical classification, material, size and cost. Refer to the equipment lists summarized in Appendix O, which characterizes the main unit operations onsite, and Appendix P, which characterizes the pumps' specifications.

3.6 Required Utilities

Four utilities are required in the proposed facility that we have designed:

- Electricity
- Compressed Air
- Natural gas
- Deionized water

Electricity is required to power most operating units in the manufacturing plant. Based on the projected energy use, the site will not qualify as a Class A facilities under the IESO guidelines and will not be eligible for Global Adjustment cost reductions [12]. As such, it will pay a blended rate of approximately $0.11/kWh of electricity used [13]. The electrical infrastructure (VFDs, transformers, etc.) required is not included in the scope of this document. The power supplied to the plant will be 3-phase, due to the size of the pumps in the facility. The exact size of the transformer required (amperage and voltage) will be determined in coordination with Hydro One once the site is developed.

Due to the explosion proof requirements of the facility, all of the tools used in the production area will be pneumatically powered. Because electric-powered tools have the potential to generate a spark, which could ignite an explosion, pneumatically-powered tools will be used to eliminate the risk of electric shock . The compressed air will be supplied to the facility using an air compressor located in the utilities building (refer to Appendix S).

Natural gas will be used to provide heating within the facility. This is greatly preferred over electrical heating due to its' overall cheaper cost. In Ontario, facilities are billed using a rate structure based on total electricity usage and on the peak electrical demand (in kW) of the facility. Because natural gas furnaces are extremely efficient, they will be able to optimize the heating expenses of the site. In Canada, natural gas furnaces are federally mandated to have a minimum efficiency of 92%, however they can be as high as 97-98% efficient in their heating [14].

Deionized water is required by the facility to slurry the reaction mixture in the Nutsche filter. The required deionized water will be produced using an on-site dual bed deionizer. The dual bed deionizer uses two tanks, one filled with an anion resin and one filled with a cation resin [15]. By running water through both of these beds, the discharged water will be free of all ions. The deionized water will be

produced in real-time based on the requirements of the current batch being run, keeping the water fresh and pure. A photo of the dual bed deionizer is shown below.

Figure 5 - A dual-bed deionizer [15]

3.7 Effluent Streams

Ensuring environmental safety and compliance is imperative to a successful plant. The effluent waste streams of the facility contain large amounts of organic solvents and other by-products. This waste cannot be simply disposed via municipal sewers and proper disposal of these effluent streams are required.

The proposed solution to this is to contain all waste products within drums, and contract a third-party company to remove the drums from site and process the waste. While this is the recommended solution, it is also recommended to explore the possibility of solvent recycling. There are companies which perform this service in the Sarnia area, like Maratek, and are contracted by large manufacturers, such as Ford [16]. Solvent recovery would effectively reduce the waste produced and would reduce the amount of fresh solvent purchased, reducing the plant's operating costs. Because large amounts of solvents are consumed throughout this process, recovering even a small percentage of the solvents used can have a large impact on the total raw materials cost. The associated costs of using this service can be found in section 7.2. As part of the scope of future work, this proposed solution should be looked into to recover solvents used onsite; however, it may not be feasible for certain solvents, like NMP, which has a very high boiling point and is reprotoxic.

3.8 Proposed Maintenance

The batch reactor and Nutsche filter will be cleaned twice every 7 weeks under reflux using toluene as the cleaning fluid. The cleaning schedule will coincide with the campaign schedule, as plant operations shift from one campaign to the next. The reactor will be cleaned using a cleaning nozzle, which can be inserted into a port in the top of the reactor and evenly sprays toluene from within the unit. Once finished, the cleaning fluid will drain into the Nutsche filter, and the same procedure will occur.

Figure 6: Batch Reactor Cleaning Demonstration Graph [17]

To ensure effective control, valves, indicators and control systems should be checked and replaced to avoid potential danger or hazards. Furthermore, a weekly visual inspection of the outdoor tank farm and chemical tanks (i.e. liquid N_2 tanks, HCl tanks) should be conducted. If any concerns are identified during these safety inspections, maintenance staff should be alerted immediately for repair.

4.0 Key Unit Analysis

Our team has identified the jacketed batch reactor as the key unit in this process.

4.1 Piping and Instrumentation Diagram

Upon determining the key unit, further analysis was performed around the reactor. A Piping and Instrumentation Diagram (P&ID) has been developed around the batch reactor for both steps of the process (refer to Appendix Q). As depicted in the P&ID, there will be a batch weighing system for solids measuring and handling, as well as storage tanks to house the liquid reagents . The main process control in the P&ID is the heating/cooling jacket of the reactor. The P&ID for step 2 looks almost identical, as most of the equipment is used for both reactions. The difference between the two processes are the reactants/solvents that are charged into the reactor.

4.2 Batch Reactor Design Parameters

The size of the reactor was determined to be 1900 US gallons (~7200 L). This was determined using the scale-up factor, cycle time, plant schedule, and production target. The reactor was sized such that both steps of the process can be performed in the same reactor. Design specifications of the reactor can be found below, with calculations in Appendix I.

The following are the design specifications for the reactor:

- Size: 1900 US gallon reactor (~7200 L)
- Height: 4.3 m
- Diameter: 1.3 m
- Material: Stainless Steel, Grade 316

A diagram of the top view of the reactor was developed to show the number and sizes of ports required in the reactor (refer to Appendix R).

The following are the ports on the top of the reactor:

- Reactant/solvent ports (x5): NMP, DMSO, DMAE, 3-PDP, solids
- Instrumentation ports (x3): pressure, temperature, level
- Nitrogen ports (x2): N_2 inlet, N_2 outlet
- Condenser port
- Pressure relief port
- Viewing port

4.3 Batch Reactor Operating Parameters

The reactor will be maintained under an inert nitrogen atmosphere. In the patented examples, only the second step occurs in a nitrogen atmosphere. However, when scaling up the process, the team decided to maintain an inert atmosphere for both steps to prevent oxidation of the reactor material. Dilution purging will be used to inert the reactor. This process involves injecting nitrogen gas to lower the concentration of

oxygen in the reactor [18]. An oxygen sensor will be installed in the reactor to ensure there is sufficient dilution before starting the reactor.

Operating temperatures for each step for the reactor are shown in the table below.
Each step of the reaction includes initial heating of the reaction mixture and subsequent cooling after the reaction has occurred. Heating and cooling temperature setpoints are dictated by the patent examples. The temperature of the reactor will be controlled using a reactor jacket.

Table 5: Predetermined operating parameters to ensure full reaction

Operating Parameters	Step 1	Step 2
Pressure	1 atm (inert with N_2)	1 atm (inert with N_2)
Temperature	30 - 90°C	25 - 180°C
Level	75% fill factor	70% fill factor

4.4 Reactor Jacket Design Parameters

The reactor will be equipped with a heating and cooling jacket to control the temperature of the reaction. Dowtherm Q was selected as the thermal fluid for the reactor jacket. This is a synthetic oil mixture of diphenyl-ethane and alkylated aromatics [19]. Dowtherm Q was selected because of its thermal stability at high temperatures.

The reactor jacket will be heated using a natural gas furnace and cooled using a cold water heat exchanger. The furnace and heat exchanger will be installed in parallel, with flow of the thermal fluid directed through the selected equipment, depending on if heating or cooling is required.

4.5 Reactor Control Systems

The P&ID for the batch reactor includes various instrumentation to measure and control the temperature, pressure, addition of reactants/solvents to the reactor.

As discussed in section 4.3, a natural gas burning furnace is used to heat the thermal fluid in the jacket, and a cold water heat exchanger is used for cooling of that oil. Cascade control will be used to control the temperature of the heating fluid. As illustrated in the P&ID, the temperature of the reacting mixture and the inlet temperature of the heating fluid will be measured. These parameters will be used to control either flowrate of the fuel to the furnace or the flowrate of the heat exchanger cooling water.

The reactor operates at a pressure of 1 atm under an inert nitrogen atmosphere for both reactions. The pressure will be measured with a pressure gauge and controlled by manipulating the pressure control valves on the nitrogen inlet and nitrogen outlet lines.

Addition of liquids is controlled by measuring liquid flowrate and manipulating flow control valves. Solid reactants are added from hoppers and the batch weighing system is used to pre-weigh the mass of required solids, manipulating the flow control valves downstream of the solid hoppers. One measured accurately, the batch weighing system releases the solids into the reactor.

4.6 Startup and Shutdown Requirements

There are various procedures that need to be followed before the startup and shutdown of this process.

4.6.1 Startup Requirements

Before startup of the process, a thorough check along the process line will need to be conducted. This check must typically occur before every batch commences operation.

Operators must ensure that the entire reactor and filters are empty before each batch is run and there is no carryover between runs. Furthermore, operators must perform a visual inspection of the pipes, valves, and pumps during each run to make sure they are functioning properly. In addition to the process lines, the storage tanks for the liquid reactants, solvents and products need to be visually inspected to check for leaks or any possible sources of contamination. Finally, the levels of reactants and solvents in each tank should be verified weekly to make sure there is enough inventory to run the scheduled 3 batches per week. If any issues arise during these visual inspections, operators are required to report their concerns to the engineers onsite or maintenance staff.

Once the preliminary checks are complete, the chemical process can begin. When charging the batch reactor, the reactants have to be added in a particular order to prevent potential hazards.

For step 1 of the reaction, charge the reactants into the reactor in the following order:

1. Add DMSO and heat the reactor to the temperature of the melted 3PDP (55°C)
2. Add the melted 3PDP
3. Add 4NPN
4. Add the anhydrous potassium carbonate
5. Inert the entire reactor and heat the reactor to 90°C

For step 2 of the reaction, charge the reactants into the reactor in the following order:

1. Add the NMP
2. Add the produced adduct, 4-(3-pentadecyl) phenoxyphthalonitrile
3. Add the DMAE
4. Add the copper (II) acetate monohydrate
5. Inert the entire reactor and heat the reactor to 180°C

4.6.2 Shutdown Requirements

To commence the shutdown procedures, operators will need to ensure that there is no reaction process ongoing in either the reactor or filter. These vessels also need to be emptied of their contents before

shutting down. Once this has been completed, all valves on the heating/cooling jacket needs to be closed. Subsequently, the furnace, condensers, pumps and heat exchangers need to be shut down and have their associated valves closed.

This shutdown procedure must be followed in cases of required maintenance, scheduled plant shutdowns and in the case of any emergency.

5.0 Plant Layout

The plant layouts were designed in compliance with industry accepted standards to the satisfaction of the client. The team has delivered four drawings to the client:

- Site layout (refer to Appendix S)
- Transport truck pathway layout (refer to Appendix T)
- 2D horizontal plant layout (refer to Appendix U)
- 2D vertical plant layout (refer to Appendix V)

5.1 2D Site Layout

Any personnel (i.e. all employees, transport truck drivers, etc.) wishing to enter the plant must pass through the security gate, as the site is gated by a security perimeter (i.e. patrolled fence). Once their access is approved, they may enter the site (refer to the full site layout detailed in Appendix S).

All transport trucks onsite require ample space to maneuver around the site. A turning radius of 180° and a minimum turning distance of 29.2 m is required by all trucks (refer to the truck turning pathway layout in Appendix T).

5.2 2D Plant Layout

Two drawings were developed to outline the plant layout - the 2D horizontal plant layout and 2D vertical plant layout.

5.2.1 Horizontal Plant Layout

Within Plant "A", the main production facility, there are two main areas - hazardous areas and non-hazardous areas. Hazardous areas are characterized as explosion-proof (i.e. XP) areas and personal protective equipment (i.e. PPE) zones on the layout (refer to the full horizontal plant layout detailed in Appendix U). All other areas in Plant "A" are non-hazardous.

5.2.1 Vertical Plant Layout

The designed chemical plant is one floor, however, the production area is operated within a multi-level section of the plant. In doing so, the design takes advantage of gravity to move fluids through the process, reducing overall energy and equipment costs for the plant (refer to Appendix V).

An operator dispenses bags of fine solids into the dispensing station on the first level, while a workstation crane dumps large quantities of bulk solids into the hoppers (i.e. T-301, T-302). The solids are then measured out into the batch weighted scale (i.e. T-201), and poured into the jacketed batch reactor (i.e. R-201), located on the second level. Once synthesized, the reaction mixture is transferred to either of the Nutsche filters (i.e. N-101, N-102), located on the first level. This process reduces the overall requirement for pumps, and effectively reduces plant utility costs.

6.0 Plant Safety Analysis

The overriding factor in the design of this plant is safety. This includes the safety of the process, personnel and environment. With a detailed analysis on these key elements, we guarantee that the proposed process will meet safety standards outlined by the federal and provincial government.

A safety summary sheet for all the chemicals used in this plant is provided in Appendix W of this report. This sheet should be consulted if any questions arise regarding the safety of a chemical. Furthermore, the plant layout in inclusive of emergency equipment locations and muster spot locations in cases of plant evacuations (refer to Appendix U).

6.1 Process Safety Analysis (PSA)

A safety analysis was conducted around process equipment in terms of various operating parameters that would have a direct, unacceptable affect on the entire process. These parameters include temperature, concentration, agitation and pressure. Using these parameters, a "what-if" analysis was conducted to look at possible scenarios that could arise along the process. Guide words such as *more*, *less*, and *none* were then employed to summarize this analysis.

Appendix X shows the results of the PSA around the jacketed batch reactor and the Nutsche filter. Shown in this analysis are the indicators for a certain safety concern, potential causes, as well as actions a plant operator can take to resolve a certain risk or safety concern.

6.2 Risks & Hazards Mitigation Strategy

Risks and hazards in this chemical production were looked into and ways in which they can be mitigated, or eliminated, were discussed. This analysis increases the safety of the MPc production, which is the main priority in the scope of work.

There are various hazards that have been identified and mitigated for the production process (refer to Appendix Y). Listed below are three important risks that have the biggest impact on the plant.

1) The different chemicals and their interaction with each other
2) Nitrogen gas used for inerting
3) Environmental pollution

The various chemicals used onsite interact differently with each other, and can impose a serious safety concern. Appendix Z references the various chemicals used and their interaction with other chemicals. One important example where this chemical interaction played a key role was in the design of the tank farm. Some of the solvents used are very reactive in the presence of a strong acid, such as the 37% concentrated hydrochloric acid. In order to mitigate this potential risk, the hydrochloric acid will be stored in a different tank farm to prevent unsafe interactions between the chemicals. Also, the nitrogen gas used for the chemical inerting of the unit operations is stored in a liquid phase away from the plant, near the product warehouse (refer to site layout in Appendix S). This building will be built with blast walls to reduce the damage a potential explosion could create.

6.3 Environmental Safety

The process for the production of MPCs has been deemed environmentally safe due to the use of green chemistry principles and the addition of various environmental safeguards [4].

In the case of any chemical spills, a containment area will be built in the tank farm and the HCl storage area at onsite (refer to Appendix S). These containment areas will have a volume of 110% of the biggest tank [20].

The volume of the tank farm will be approximately 30 m^3 (29.56m^3), yielding the containment area to have dimensions of 20.7 m x 11.5 m x 0.13 m. The HCl storage area will have an area of 2.91m^3, yielding the containment area to have dimensions of 3 m x 3 m x 0.33 m. The containment areas will be constructed using a synthetic liner so that the spill cannot escape and contaminate the soil in the local environment.

The plant will also have spill kits for fast cleanup of small, contained spills and/or leaks. The spill kit will contain safety goggles, gloves, disposable bags, pads and socks. Plant operators will be responsible for using spill kits to clean up potential spills around the plant. These emergency spill kit locations are referenced on the site and plant layouts (refer to Appendices S and U). Furthermore, a CO_2 monitor will also be installed in the plant to detect gaseous leaks of rising CO_2 concentrations in the air.

With all these safeguards in place, it is guaranteed that the plant will be run as safely as possible.

6.4 Required Personal Protective Equipment (PPE)

The production facility, like most chemical processing sites, has a PPE designated zone, where required PPE must be worn at all times. Appendix U shows the designated PPE areas located within the plant where the following PPE are required:

- Head Protection: Hard hat, Type 2, Class C hard hat [21]
- Eye Protection: Clean, safety glasses with side shields
- Body Protection: Chemical protective clothing, especially for workers handling the solid reactants, check safety summary sheet (refer to Appendix W)
- Hand Protection: Appropriate chemical resistant gloves when handling chemicals, consult safety sheet summary (refer to Appendix W)
- Foot: Steel toe boots

Although NMP is reprotoxic, there is no need for operators to wear respirators. As the NMP is contained and operators have no contact with NMP during normal operation of the chemical plant, the exposure risk is minimized. However, in the case of a spill or plant shutdown, all personnel will need to wear a full face respirator with multi-purpose combination for safety.

6.5 Visitors Safety Management Plan

As safety is our top priority, the team has identified a potential safety risk with visitors onsite. Contractors, consultants and sampling technicians are all examples of individuals that may frequent the site and impose a threat to their well-being and the safety of those around them. Being that they are not trained employees, we cannot expect them to be familiar with safe manufacturing practices. Creating a Visitors Safety Management Plan will reduce the risk imposed by any visitors.

Visitors that wish to enter the site will need to sign in at the security gate before entering (refer to Appendix AA). This will ensure that everyone onsite can be accounted for in case of an emergency.

Before entering the chemical processing plant, visitors will be acquainted with the plant's safety practices and policies, plant expectations, plant layout, and mandatory safety precautions. A safety video encompassing these topics will be available for all visitors in order to acquaint themselves with the plant safety policies. This minimizes unsafe practices and reduces the liability of the production facility.

Upon entering the plant, all visitors will be provided with the required PPE and accompanied by a host. All PPE is located in the "Supplies Stores" in the plant (refer to Appendix U). The host must be a plant employee, trained in safe manufacturing practices and well-acquainted with the perimeter of the site. In the case of an emergency (i.e. fire, spill, etc.), the host will be responsible to lead the visitor to a safe assembly point (refer to Appendix U).

When visitors are ready to leave the site, they must exit through the security and sign out on the visitor log book. In doing so, everyone will be accounted for and get home safely at the end of the day.

7.0 Economic Analysis

An economic analysis was performed to determine the economic viability of this project. This includes a breakdown of the total fixed capital cost, annual manufacturing cost, and annual sales revenue. With that, a cash flow diagram was created for the project. Finally, the net present value was calculated to determine the profitability and payback period of the project.

7.1 Total Fixed Capital Cost

The total fixed capital cost is estimated at $22.95 million dollars. The major contributing costs are the equipment cost, construction cost, and working capital.

To estimate the cost of land, a similar piece of land was sourced in Sarnia, ON (refer to Appendix AE). To scale this piece of land to the correct size required, the following formula was used [22]:

$$Land/Equipment\ Price = (Price\ of\ Similar\ Land/Equipment) \times (\frac{New\ Capacity}{Previous\ Capacity})^n$$

In the equation above, n represents the index factor, which typically follows the 6/10th rule; therefore, n is 0.6 [22].

To account for inflation, the current price of equipment was calculated using the following formula:

$$Current\ Price = (Price\ in\ a\ Given\ Year) \times (\frac{Current\ Cost\ Index}{Cost\ Index\ for\ a\ Given\ Year})$$

Equipment Free On Board (FOB) costs are provided by the equipment suppliers. To account for installation and delivery fees, the equipment FOB costs were multiplied by a factor of 4 (refer to Appendix AD). The construction cost of the plant was estimated based on the cost of the explosion-proof (XP) area, undeveloped area, and the tank farm area (refer to Appendix AE). Based on the team's working hours (refer to section 1.2, Appendix B), a one-time consulting fee was included. A working capital is also required to initiate the production process. For this project, two months worth of the raw materials will be purchased to begin plant operations.

The total fixed capital cost was estimated using the Szabo Heuristic method. This is to account for the cost of engineering supervision, contractor's fees, and contingency fees that should be considered in the construction of a new plant. The Szabo Heuristic method is as follows:

$$Fixed\ Capital\ Investment = (2.86 \times Equipment\ Cost) + (1.3 \times Construction\ Cost) + (1.3 \times Land\ Cost)$$

The fixed capital cost was then calculated (refer to Appendix AF). A total breakdown of the components are listed in table 6, and shown in figure 7.

Table 6: Breakdown of the total fixed capital cost estimated using Szabo heuristics

Components	Cost
Equipment Cost	$4,820,485
Land Purchasing Cost	$386,350
Construction Cost	$4,749,954
Working Capital	$2,481,760
Engineering Consulting Fee	$22,692
Contingency, Engineering Supervision, utilities, auxiliary facilities Fees	$10,484,303
Total Fixed Capital Cost	$22,945,544

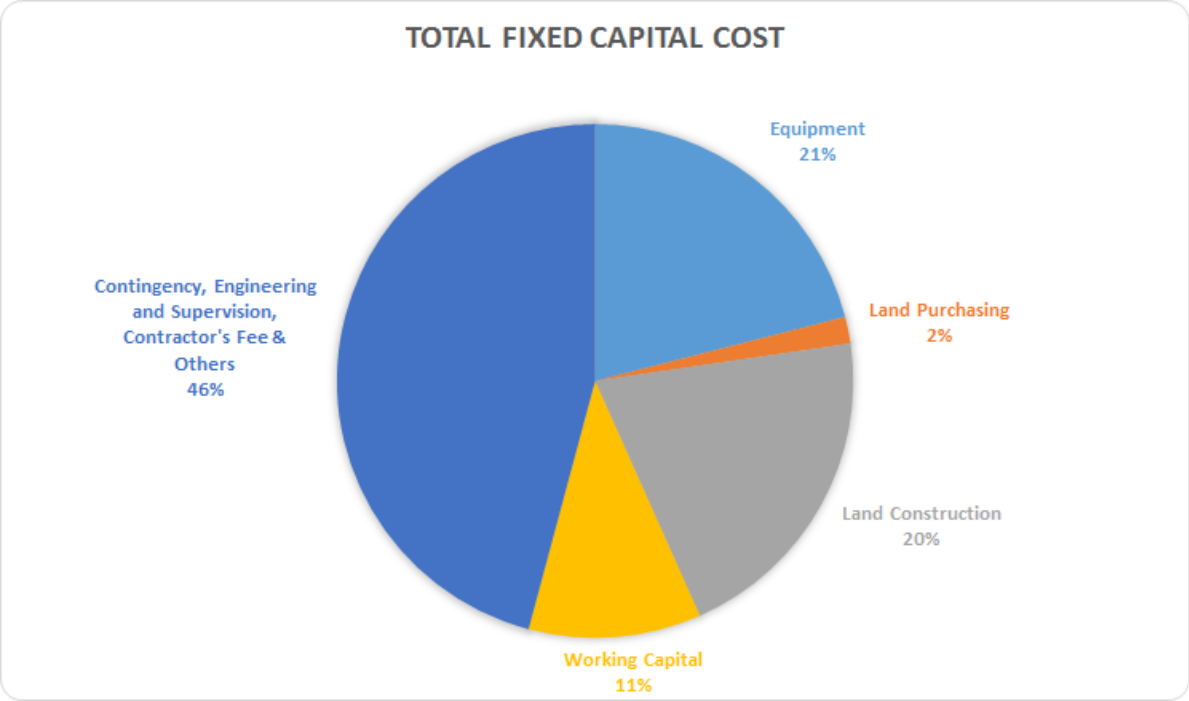

Figure 7: Segregated segments of total capital costs

7.2 Annual Manufacturing Cost

The annual manufacturing cost is estimated at $20 million dollars. This cost is composed of the raw material costs (RMCs), maintenance fees, labor and staff salaries, payroll, plant overhead cost, utilities cost, waste disposal cost, taxation and insurance, sales associated, and supplies cost. A breakdown of these components is included in table 7 and figure 8.

Raw material costs were calculated based on the yearly production target, required chemicals, and their corresponding masses and costs (refer to Appendix AC). The industrial price of chemicals were provided from the suppliers. This includes the cost of insurance and freight (CIF). The cost per kilogram for the production of the final product is $261. This was calculated based on the CIF cost (refer to Appendix AC). This cost was then scaled up to the industrial production rate, 50,000 kg/year, resulting in a $13 million RMC per year.

Due to large equipment requiring cleaning and possible repairs and also possible replacements for smaller equipments, an annual maintenance fees was calculated. The maintenance fees have been estimated to account for 6% of the fixed capital cost.

Staff salaries are identified as either direct or indirect labor costs. Direct labor costs are associated with the operators of the facility, those who work on the assembly line and monitor equipment such as the reactor, the Nutsche filters, and any solids handling. Employees will be rotated per shift; there will be 3 shifts, each 8 hours long. The indirect labor costs are associated with support workers who help in the production of the MPcs.

Direct Labor Cost

The number of operators per shift is calculated using the following formula:

$$N_{OL} = (6.29 + 31.7P^2 + 0.23N_{np})^{0.5}$$

- N_{OL} is the number of operators per shift
- P is the labor associated with solid transportation or solid discharging (i.e. $P = 0$)
- N_{np} is the labor associated with any important equipment (i.e. operators will be required for the batch reactor, nutsche filters, and control room)

Based on this formula, 3 operators are required per shift. A factor of 4.5 is applied to determine the total number of operators required per day, resulting in a total of 14 operators (refer to Appendix AB).

Indirect Labor Cost

With regards to indirect labor costs, the following positions are identified:

- QA/QC Technician (1), for quality control and testing,
- Shift Supervisor (1 per shift, 3 total)
- Managers (3) to act as plant manager, human resources, marketing manager
- Administrative Assistant (1)
- Health and Safety Officer (1)

Salaries for each position have been identified, and a factor of 20% was applied to account for CPP, vacation pay, and EI (refer to Appendix AB). Supervisor and manager salaries account for the plant overhead costs. These are minimized to ensure efficient operation of the plant.

The required utilities are electricity, compressed air, natural gas, and deionized water (refer to section 3.6). The required amount of natural gas and deionized water were calculated using the mass and energy balance. The electrical requirements of the facility were determined by looking at power requirements of the largest components (i.e the Nutsche filters) and by comparison looking at the power requirements of a similarly sized facility.

The waste is composed of solid and liquid organic mixtures. The total annual waste disposal cost is estimated based on the waste disposal cost per mass of waste (refer to Appendix AG).

For taxation and insurance, a factor of 2% is applied to the fixed capital investment.

Cost for sales associates is approximated as 4% of the products' revenue, as salespeople are generally paid on commision.

Direct supplies include items employees require to perform their work. This includes personal protective equipment (PPE), computers, and other office supplies. This correlates to the number of operators and other administrative staff, as well as their salaries. As a result, a factor of 30% of operating labor cost is used to estimate direct supply cost.

Table 7: Manufacturing Cost Breakdown

Content	Cost per Year
RMC	$13,061,896
Operating Labor Cost	$770,000
Maintenance	$1,378,094
Local Taxation	$459,365
Insurance	$229,682
Direct Supplies (PPE, office supplies)	$231,000
Overhead Plant Cost	$571,262
Sales Associated Cost	$1,400,000
Payroll	$268,252
Nitrogen	$28,098
Utilities	$384,840
Waste Disposal Cost	$988,992
Total Manufacturing Cost	$19,771,481

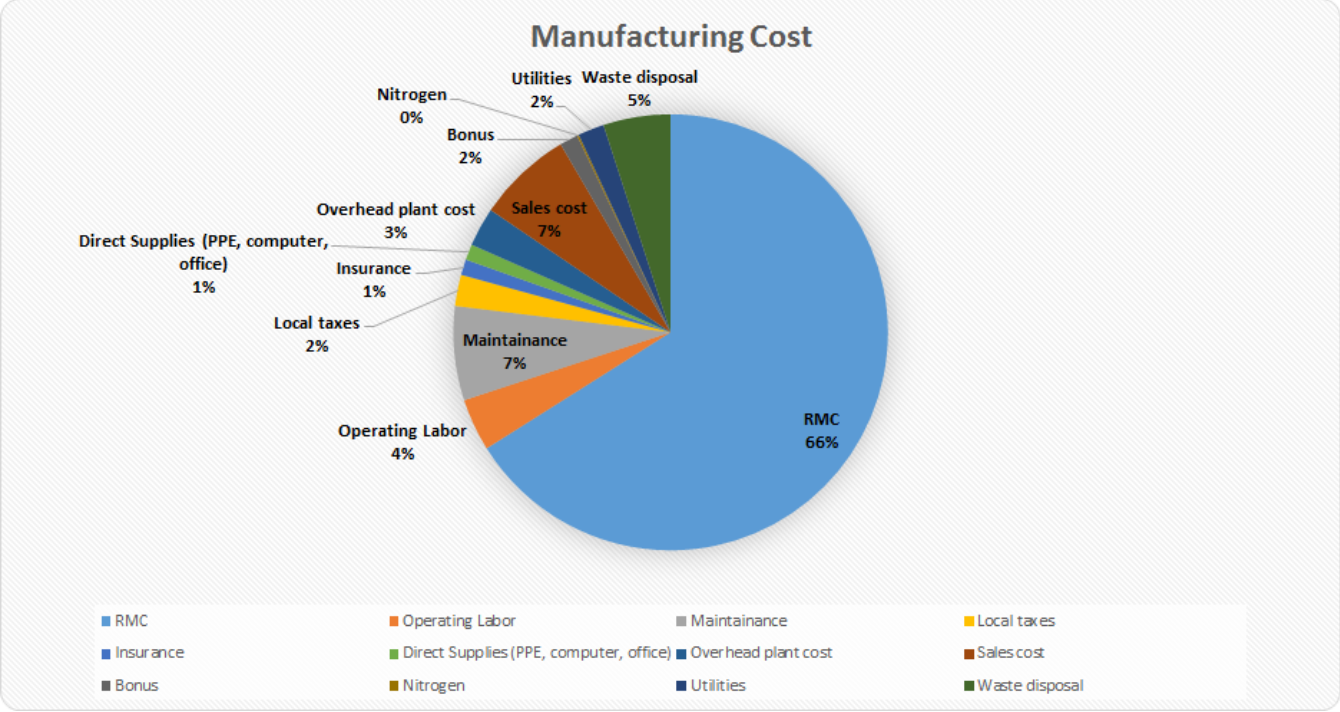

Figure 8 Segregated segments of annual manufacturing cost

7.3 Annual Revenue

The proposed sales price of the phthalocyanine dye is $525 CAD/kg and the total proposed revenue is $26.25 million dollars/year. This recommendation is based on the payback period and cash flow. A sensitivity analysis was performed around 80% to 120% of the recommended product price to determine the optimal payback period. In addition, the internal rate of return was adjusted to achieve a cumulative $0 CAD in accumulated cash flow at a payback period of 5.5 years.

7.4 Cash Flow Analysis

A cash flow analysis was performed to determine the payback period based on the initial fixed total capital investment, annual manufacturing cost, and annual sales revenue. Depreciation and taxation are considered in the cash flow analysis. A depreciation factor of 30% is applied with the half-year rule. This results in 15% depreciation in the first year and 30% over the next 4 years. The taxation rate is 45% of the annual net income of the project. The Minimum Acceptable Rate of Return (MARR) is set to 10%, and the following formula is used to calculated cumulative net present value of the project:

$$Net\ Present\ Value = \frac{FutureValue}{(1+MARR)^n}$$, where n is the time period

A payback period of 5.5 years was identified based on the cash flow diagram.

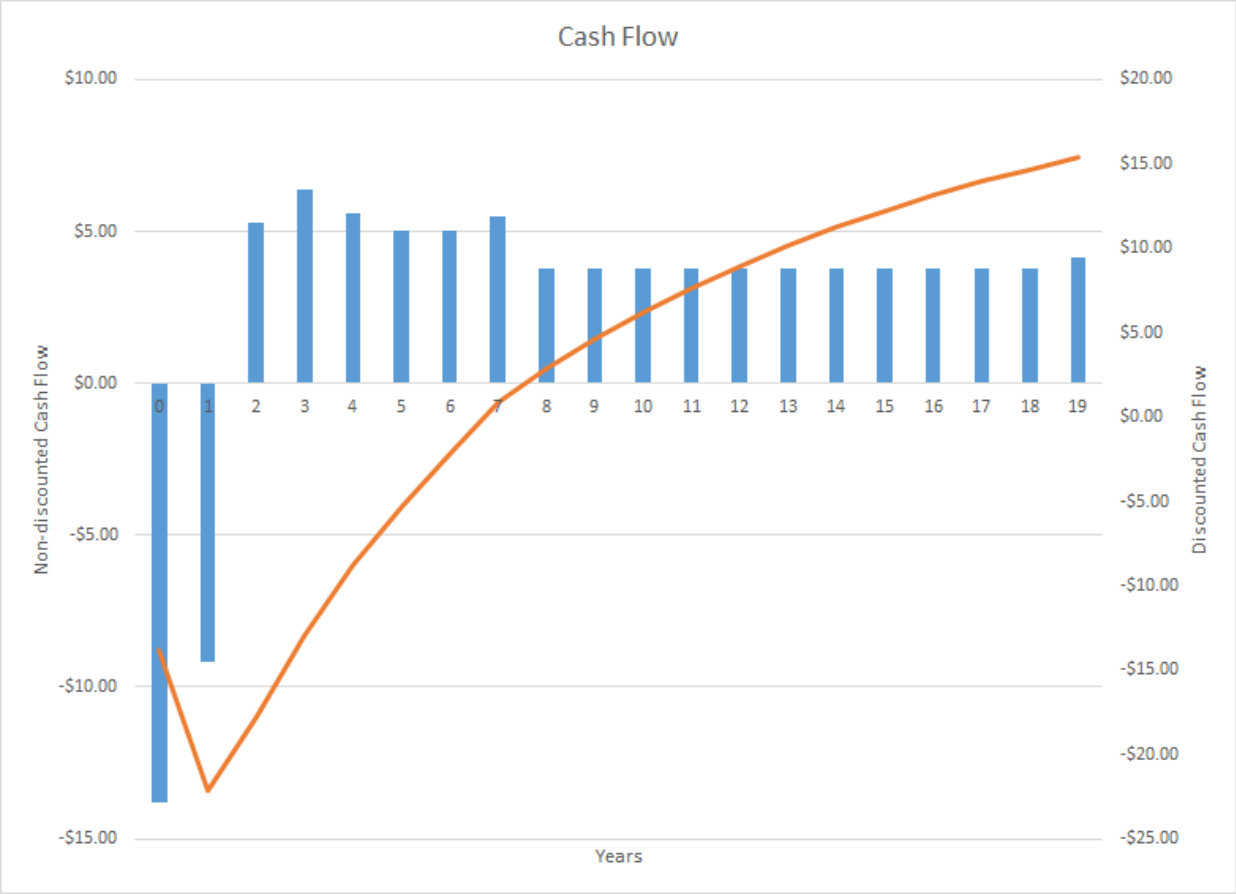

Figure 9: Cash flow diagram of project

7.5 Sensitivity Analysis

A sensitivity analysis was performed to determine the sensitivity of the net present value following changes in sales cost, manufacturing cost, and total fixed capital cost. For the base case, the net present value is $15.45 million. The variables that affect the net present value are revenue (majorly dependent on sales price), manufacturing cost, and total fixed capital cost. For the sensitivity analysis, the price of these variables is reduced or increased by 20% to observe the effects on the net present value. As seen in figure 10, the net present value is most sensitive to revenue. When sale price is reduced by 20%, the net present value becomes negative. When sale price is increased by 20%, the net present value increases to $38.7 million. Manufacturing costs also affects the net present value, but to a lesser extent. Total fixed capital cost has little influence.

Figure 10: Tornado Chart for Net Present Value Sensitivity Analysis

The sensitivity of the total manufacturing cost was also evaluated. Variables affecting manufacturing cost are raw materials, operating labor, overhead, and sales-associated costs. As seen in figure 11, the manufacturing cost is most sensitive to the raw material cost. Operating labor, overhead, and sales costs do not have a significant impact on manufacturing cost.

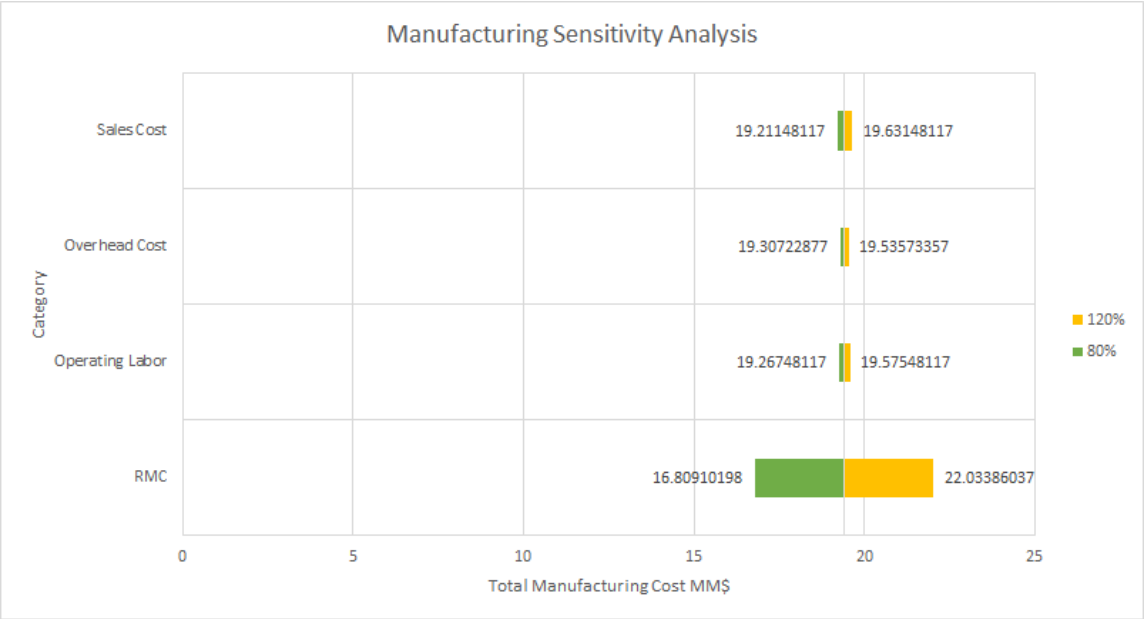

Figure 11: Tornado Chart for Manufacturing Cost Sensitivity Analysis

To increase the profitability of the plant, two options are evaluated: increasing revenue by proposing a higher MPc sale price, or decreasing manufacturing cost by decreasing RMC. Increasing the revenue will reduce the payback period, but may result in a decrease in sales. To decrease RMC, investigation to reduce the price of 4NPN is recommended as this is the most expensive raw material (refer to Appendix AC).

7.6 Internal Rate of Return

For the plant lifespan of 20 years, the internal rate of return (IRR) is equal to 22%. The typical MARR value is 5%-10%. Since the IRR is greater than the MARR, the project is economically feasible.

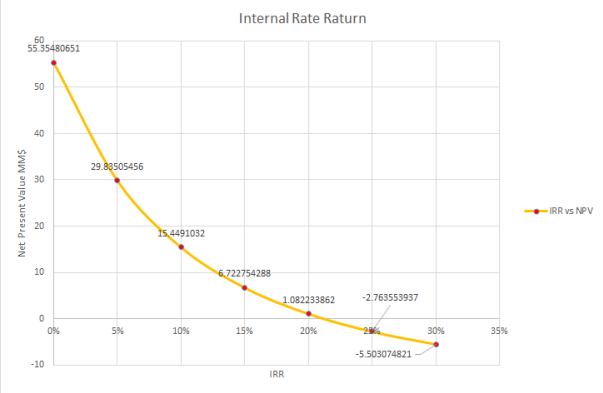

Figure 12: Net Present Value Versus Internal Rate of Return

8.0 Environmental Constraints

According to the federal government's Greenhouse Gas Reporting Program (GHGRP), all manufacturing facilities that emit over 10,000 tonnes of greenhouse gases (GHGs) in CO_2 equivalent units per year must submit a report and are subject to federal regulations around the reductions of GHGs [23]. Based off of the site's natural gas usage and CO_2 equivalence factor [24], we determined the annual CO_2 emissions from the equipment to be 8.4 tonnes and from the synthesis reaction in the batch reactor to be 7.7 tonnes. Upon a preliminary evaluation of the GHGs emitted from our site, our team determined our emissions to be approximately 16 tonnes of CO_2 equivalent units per year, making our facilities a non-reportable site.

The site was built in compliance with the following environmental regulations:

- In the case of a spill, all spill response plans should be in compliance with Ontario Regulation 675/98 [24]. Engineering staff will be responsible for developing, maintaining and reporting on the site's spill response plans.
- All aqueous waste disposed of down sewer drains must be in compliance with Ontario Regulation 169/03: Ontario Drinking Water Quality Standards [26]. As a result, our site will contract Maratek to dispose off all waste in a safe manner [16]
- During production, noise emitted must be within the acceptable range for a manufacturing facility as dictated by Ontario Regulation 381/15 [27]. Because the site is not located near residential areas, noise is not a large concern.

9.0 Legal Requirements

Our team built the site in compliance with the following regulations:

- Legal lifting weight for operators must be less than 51 lbs (23 kg) [28]. Operators won't lift anything heavier than 22 kg, which is the weight of the solids chemical bags delivered onsite

10.0 Engineering Recommendations

Upon the completion of our design, our team has recognized gaps in the proposed solution and have identified these concerns as areas for future work:

- Negotiate contract prices with Maratek to recover solvents for reuse
- Negotiate lower RMC, in particular 4NPN, with suppliers
- Perform laboratory analysis to optimize patented solution (i.e. reduce the amount of solvent required, reduce the amount of time required for slurries and drying). For example, if the slurry time in the Nutsche filter increased, the volume of the Nutsche filter would decrease dramatically, reducing the equipment cost of the most expensive units
- Perform laboratory analysis to determine the thermodynamics of reaction
- Perform laboratory analysis to eliminate the use of NMP, a reprotoxic solvent

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13.0 Appendices

Appendix A - Gantt Chart

Our team utilized the Gantt chart as a tool to plan, track and measure our completed progress. Referenced below are the Gantt charts that have been continuously updated throughout the course of our design project.

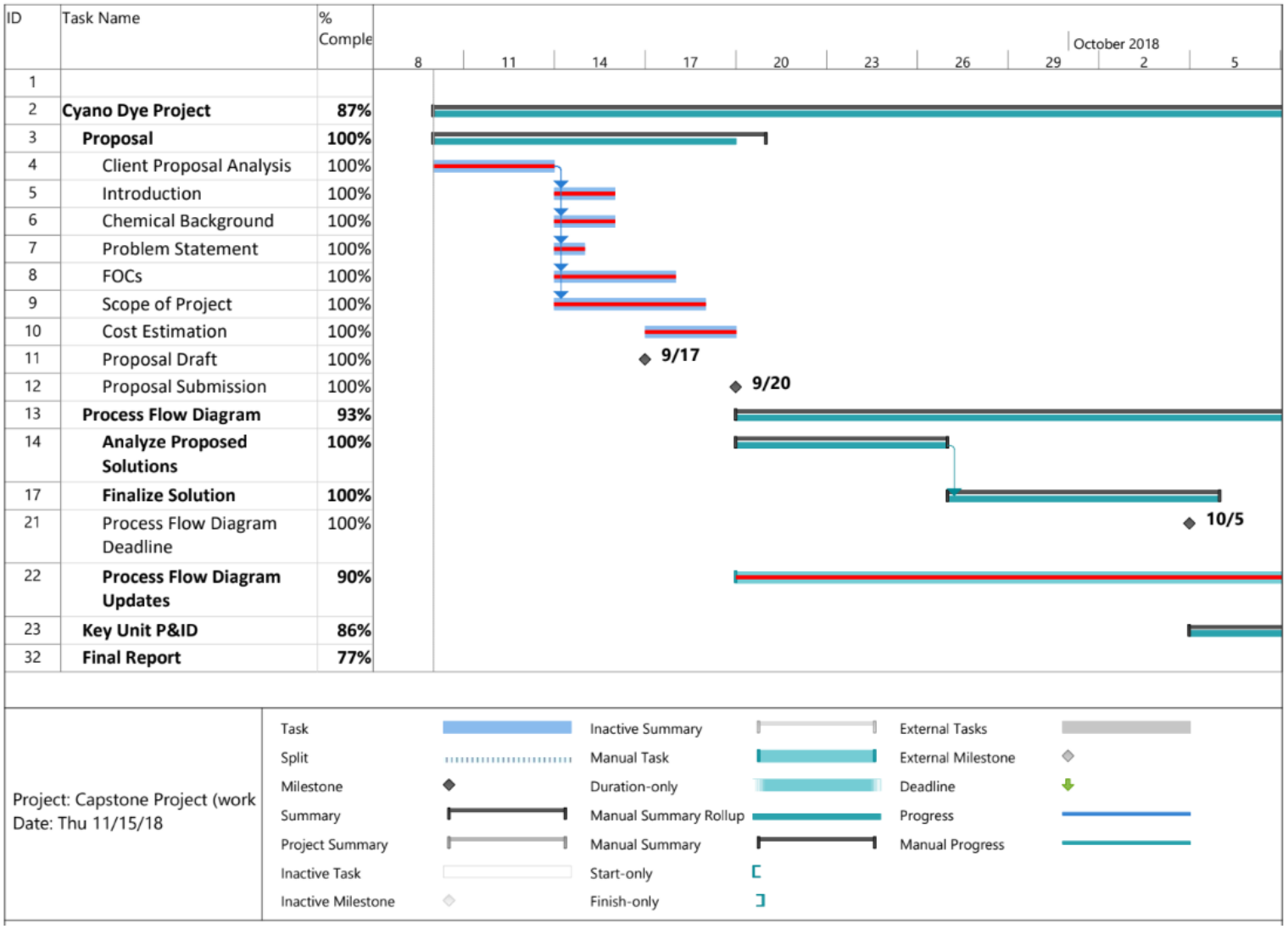


Figure A1: The above Gantt chart illustrates the first half of project schedule

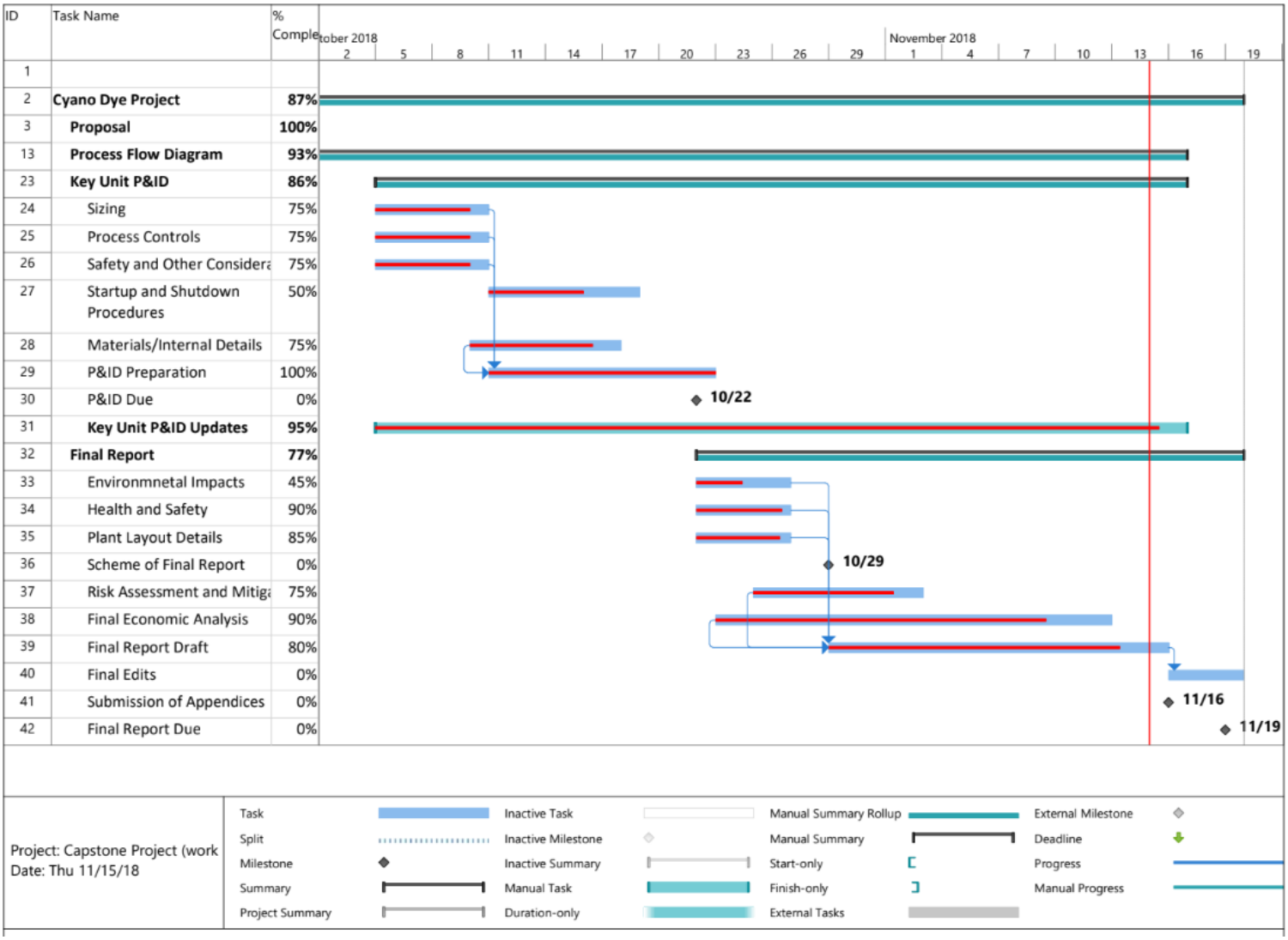


Figure A2: The above Gantt chart illustrates the second half of project schedule

Appendix B - Time Log

As shown below, the team has contributed 610 working engineering hours to the completion of this design project.

Assuming an average engineering salary in Canada to be $31.00/hour [A1], and a profit margin of 20%, the total engineering cost of this project was calculated as follows:

Total engineering expenses = $31.00/hour * 610 hours *1.20 = $22,692 CAD

Therefore, our team has billed our client approximately $23,000 in engineering expenses.

Table A1: A weekly summary of the hours contributed to the design project by each team member

Team Member	Total Hours Worked	Hours Worked per Week									
		9/10/ 2018	9/17/ 2018	9/24/ 2018	10/1/ 2018	10/8/ 2018	10/15/ 2018	10/22/ 2018	10/29/ 2018	11/5/ 2018	11/12/ 2018
Nyat Habtit	124.5	8	10	13	14	11	12	17	10.5	14	15
Anita Ankisetty	122	7	9	12	14	12	12	16	12	13	15
Jeff Dryden	123.5	7	9	12	14	12	13	16.5	11	14	15
Claude Nnadi	122.5	7	9	12	14	11	12	15	13	14.5	15
Henry Wu	117.5	7	9	12	14	11	12	15	9.5	13	15
Team Total	610	--									

Appendix C - SNAr Reaction

The following chemical process summarizes the SNAr reaction that occurs in step 1 of the outlined process. The SNAr reaction produces the intermediate product, the metallic phthalocyanine adduct.

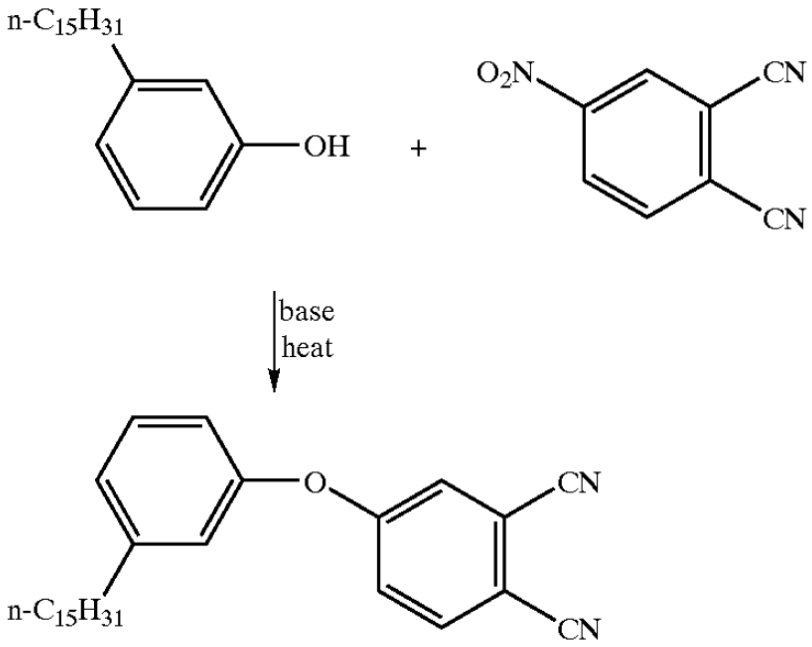


Figure A3: Reaction of 3-n-pentadecylphenol and 4-nitrophthalonitrile in the presence of a base to form the metallic phthalocyanine (MPc) adduct [A2]

Appendix D - Formation of Phthalocyanine

The following chemical process summarizes the synthesis reaction that occurs in step 2 of the outlined process. This process produces the final product, the alkylphenoxy- metallic phthalocyanine dye.

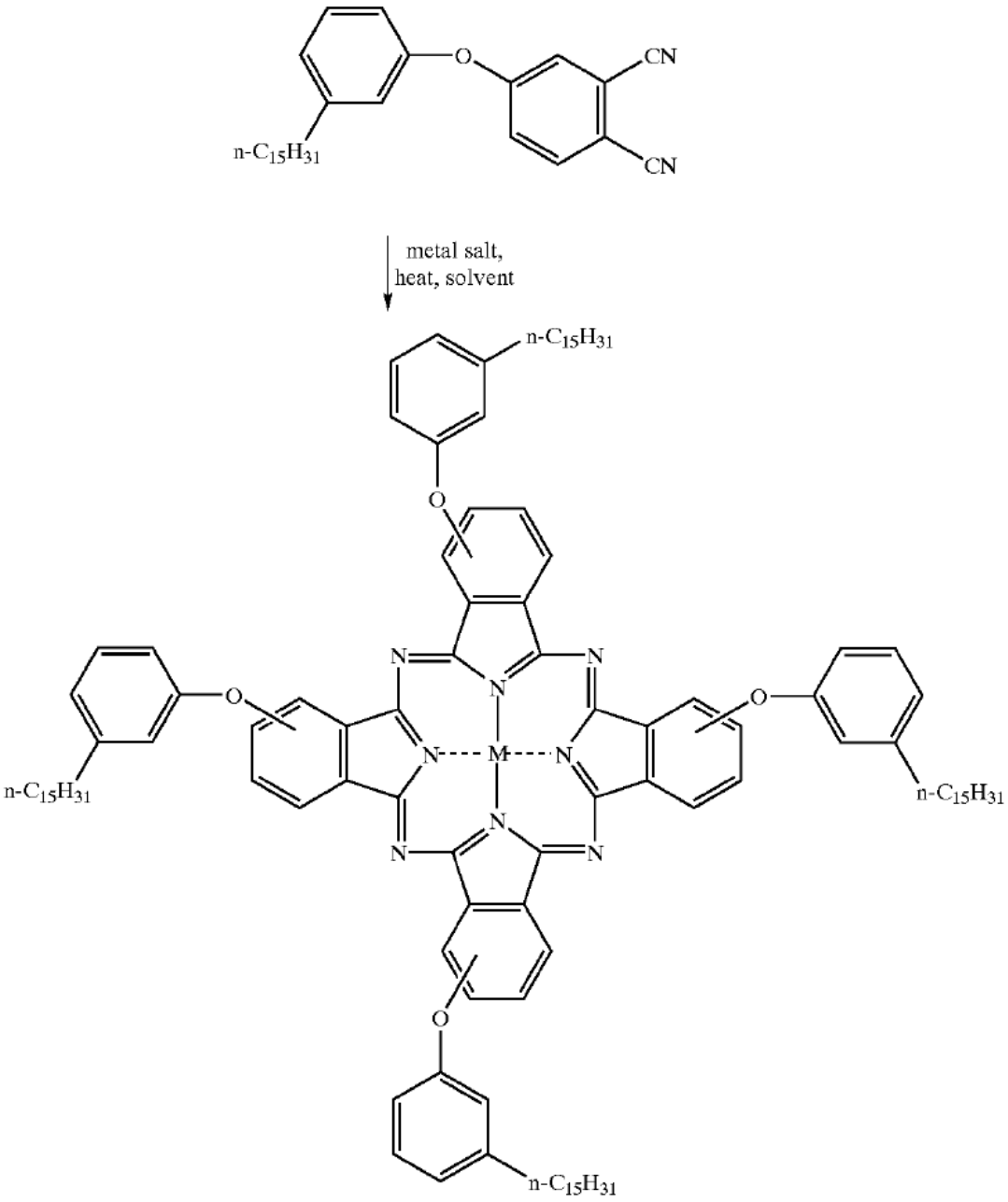


Figure A4: Addition of metal compound to the MPc adduct for formation of the alkylphenoxy-MPc colorant [A2]

Appendix E - Site Location

The site, as specified by the client, will be located in the chemical sector of Sarnia, ON. The proposed site has an area of 0.02 km^2 (5 acres). It is located at 42°56'39.7"N 82°22'43.7"W, and is referenced below.

Figure A5: A screenshot of the proposed site in Sarnia, ON [A3]

Appendix F - Preliminary Raw Material Cost (RMC) of Patented Examples

Preliminary raw material costs were calculated and used to evaluate the patent examples. A summary of these costs and an evaluation of the patent example can be found in the tables below.

Table A2: RMC for patent examples 1 to 4, for step one of the process.

Example in Patent	Raw Material Cost (CAD)	Evaluation
1	$123.5/kg [A4, A5, A6, A13]	Step 1 of the overall reaction with high yield, 87.6%, and high purity, 97%.
2	$146.6/kg [A4, A6, A7, A9, A14]	Step 1 of the overall reaction with high yield, 98%, but low purity, 67%.
3	$106.2/kg [A4, A5, A6, A9]	Step 1 of the overall reaction with high yield, 84%, but low purity, 89%.
4	$135.97/kg [A4, A5, A6, A7, A8, A9]	Step 1 of the overall reaction with 90% yield and 98% purity.

Table A3: RMC for patent examples 5 to 8 and 11 to 14, for step two of the process. Examples 11 to 14 were not evaluated as they did not meet the design objectives.

Example in Patent	Raw Material Cost (CAD)	Evaluation
5	$475.7/kg [A5, A9, A11, A19]	Step 2 of the overall reaction with yield 45%, the reaction does not use catalyst.
6	$256.2/kg [A12, A15, A19]	Step 2 of the overall reaction without catalyst, the yield is 56%; and it is dark blue, waxy globular lumps, which is difficult to purify.
7	$135.9/kg [A12, A14, A15, A19]	Step 2 of the overall reaction with ammonium acetate catalyst, it has 2 heating stages and releases ammonia gas. It produces 98% purify coarse powder.
8	$92.2/kg [A15, A16,	Step 2 of the overall reaction with purity 98% and produce coarse dark blue powder

	A19]	
11	N/A	Step 2 reaction to produce zinc dye, the product is a sticky solid with 56% yield.
12	N/A	Step 2 reaction to produce non-metallic MPc, produces lumps of dark blue, gummy solid with 19% yield.
13	N/A	Step 2 reaction to produce nickel dye, the product is sticky globular solid with 49% yield.
14	N/A	Step 2 reaction to produce cobalt dye as sticky balls and it has low yield, 34%.

Table A4: RMC for patent examples 9 and 10, for the one-step full process.

Example in Patent	Raw Material Cost (CAD)	Evaluation
9	$166.0/kg [A4, A5, A6, A9, A14, A15, A19, A20]	Full reaction with low yield, 41%, it has no methods to wash or purify intermediates and produces bluish black solid.
10	$130.3/kg [A4, A5, A6, A12, A15, A19, A20]	Full reaction with 67% yield and 86% purity, and the property of the product is dark blue powder.

Appendix G - Decision Making Matrices

Various decision making matrices were developed to evaluate the patent examples and select the optimal process for step one and two of the reaction. Table A5 evaluates patent examples 1 to 4 for the first step of the process. Table A6 evaluates patent examples 5 to 8 for the second step of the process. Table A7 evaluates examples 9 and 10 for the one-step reaction. Patent examples 11 to 14 were removed from the scope of this evaluation as they did not meet the objectives of the design, as described in Appendix F.

Each criteria was assigned a colour (red, yellow, or green) to help compare the examples. Red indicates a risk, or undesirable component of the process, yellow indicates a satisfactory component and green indicates a desirable component.

Table A5: Decision making matrix for examples 1 to 4 of the patent. These address the first step of the two-step process.

Example & Solvent	Toxicity / Occ. Health	Safety	Cost	Purity	Yield
#1 (NMP)	OEBV4 G2 Sk	SHB3	$124/kg	97%	87.6%
#2 (DMF)	OEBV4 G2 Sk	SHB2	$147/kg	67%	98%
#3 (NMP)	OEBV4 G2 Sk	SHB3	$106/kg	89%	84%
#4 (DMSO)	OEBV2 Sk	SHB4	$136/kg	98%	90%

Table A6: Decision making matrix for examples 5 to 8 of the patent. These address the second step of the two-step process.

Example & Solvent	Toxicity / Occ. Health	Safety	Cost	Purity	Yield
#5 (Hexanol)	OEBV3 Sk	SHB3	$476/kg	—	45%
#6 (NMP)	OEBV4 G2 Sk	SHB3	$256/kg	waxy, globular	56%
#7 (NMP)	OEBV4 G2 Sk	SHB3	$136/kg	~98%	74%
#8 (NMP)	OEBV4 G2 Sk	SHB3	$92/kg	~98%	80%

Table A7: Decision making matrix for examples 9 and 10 of the patent. These represent a one-step process for synthesis of MPc.

Example & Solvent	Toxicity / Occ. Health	Safety	Cost	Purity	Yield
#9 (NMP)	OEBV4 G2 Sk	SHB3	$166/kg	fine solid	41%
#10 (NMP)	OEBV4 G2 Sk	SHB3	$130/kg	86%	67%

Tables A8 and A9 evaluate the feasibility of producing one of the key reagents in the process, 3-pentadecylphenol, in-house through the hydrogenation of cardanol or to purchase it on the market.

Table A8: Decision making matrix for in-house hydrogenation of cardanol.

Substance Name	Personnel & Env. Safety	Cost	Toxicity / Health Effects	Comments
Cardanol	1	$350 [A20]	2	Acute toxicity if inhaled, contact, oral. Skin/eye irritant - require PPE (mask, eyeshield, gloves)
Catalyst (Ni-Al)	2	$4,630 [A21]	3	Health hazard, acute toxicity - requires PPE (respirators, eyeshields, gloves), flammable solid
Nitrogen Gas	2	$15,810 [A22]	2	Explosive - safety concern. Not toxic in air at low concentrations.
Hydrogen Gas	3	$310,070 [A23]	-	Extremely flammable/explosive - safety concern

Table A9: Decision making matrix for the purchasing of pre-made 3-pentadecylphenol

3-Pentadecyl-phenol	1	$179,900 [A4]	2	Acute toxicity if inhaled, contact, oral. Skin/eye irritant - require PPE (mask, eyeshield, gloves)

Appendix H - Mass Balance

Table A10: Mass balance for step 1, based on the block flow diagram referenced in section 2.1 of the report. Step numbers correspond to blocks in the BFD.

STEP 1	Streams 1-5		Stream 6		Stream 7 (x2)		Stream 8		Stream 9 (x2)		Stream 10 (x2)		Stream 11	
(kg/batch)	IN	OUT	IN	OUT	IN	OUT	IN	OUT	IN	OUT	IN	OUT	IN	OUT
3-PDP	1000													
DMSO	3980													
K2CO3	398													
4-NPN	498													
Adduct & Impurities		5876	5876	1852	1852	1852	1852	1852	1852	1852	1852	1852	1852	
Deion. H2O			5970		11940				11940					
HCL							12038							
Methanol											12609			
Waste				9994		11940		12038		11940		12609		741
MPc Adduct														1111

Table A11: Mass balance for step 2, based on the block flow diagram referenced in section 2.1 of the report. Step numbers correspond to blocks in the BFD.

STEP 2	Streams 1-6		Stream 7		Stream 8		Stream 9		Stream 10	
(kg/batch)	IN	OUT	IN	OUT	IN	OUT	IN	OUT	IN	OUT
MPc Adduct	1110									
NMP	3667				2805					
DMAE	114									
Copper Acetate	114									
MPc & Impurities		5005	5005	1339	1339	1339	1339	1339	1339	
Methyl Ethyl Ketone (MEK)							5291			
Waste				3666		2805		5291		536
MPc Final Product										803

Appendix I - Reactor Sizing Calculations

The following are a list of assumptions that were used to calculate reactor size for step 1 and 2:

- Assume the density of the mixture is equivalent as the density of the solvent
- Assume a 99% process efficiency
- Assume a 1% yield losses
- Assume a fill factor of 75% - 85% when calculating reactor volume

The following iterative process was used to size the reactor:

1. Assume a scale-up factor (SUF):

$$SUF = \frac{(scaled\ up\ mass\ of\ 3\text{-}PDP)}{(patent\ mass\ of\ 3\text{-}PDP)}$$

2. Calculate reactor volume required for the scaled up mixture:

$$V = \frac{(total\ mass\ of\ reactants\ \&\ solvents) \times SUF}{(density\ of\ solvent) \times (fill\ factor\ \%)}$$

3. Calculate production per batch:

$$product\ per\ batch = (patent\ mass\ of\ product) \times SUF$$

4. Calculate production per year, based on the scale up factor determined in step 1:

$$production\ per\ year = production\ per\ batch \times batches\ per\ week \times plant\ uptime\ (weeks\ per\ year)$$

6. Iterate:
   - Compare calculated production per year and required production per year.
   - Modify scale up factor until these are equal.

Table A12: Results of reactor sizing calculations for step 1 and 2

Parameters	Step 1	Step 2
Scale-up factor (SUF)	~ 1990	~ 182567
Fill Factor	75%	70%
Reactor Volume	1900 US gallons	1900 US gallons
Product per batch	1111 kg	803 kg
Mass of product produced per year	70,008 kg	50,607 kg

Appendix J - Condenser Sizing

Assumptions in sizing the condenser on top of the jacketed reactor (i.e. C-201):

- Assume the reaction does not raise the temperature of the overall mixture
- Use the cleaning process of the jacketed reactor to size the condenser. Assume the cleaning fluid to be toluene
- Assume the reactor will be filled to 75% of it's capacity with toluene and refluxed at 110°C
- The area of the condenser was sized using a heuristic calculation, in which the area of the condenser is equivalent to the volume of the batch reactor (1900 U.S Gallons is equal to 7.19 m^3)
- To ensure that the condenser can provide enough cooling for this reflux, match the energy provided by the condenser towards the toluene vapors to the energy provided by the heating jacket to the toluene. Use the following equation to do so - Q=UA(Ts-T)

Table A13: Parameters contributing to the energy balance around the condenser, C-201

Parameter	Value
Temperature of the Heating Jacket (assumed isothermal)	150°C
Boiling Temperature of Toluene	110°C [A24]
Area of the reactor at 75% fill	16.14m^2
Thermal Conductivity of the Heating Jacket and Condenser	300 W/m2*K
Power provided by the Heating Jacket	Q = 300*16.14*(150-110) = **194 kW**
Area of the condenser	7.1 m^2
Average Temperature of the Condenser	20°C
Assume Temperature of the Toluene Gas	110°C
Power provided by the Condenser	Q = 300*7.19*(110-20) = **194 kW**

Since the energy provided by the heating jacket matches the energy provided by the condenser, the condenser is appropriately sized.

Appendix K - Energy Balance

The following is a list of assumptions that were made to calculate the energy balances around the jacketed reactor for both steps 1 and 2:

- The energy released during the reaction is equal to the energy lost to surroundings
- The reactor (i.e. R-201) has an overall heat transfer coefficient (i.e. U value) of 300W/m^2*K
- The volume of the jacketed reactor is 1900 U.S. gallons
- The ratio of height to diameter of the reactor is 3:1
- The reactor is considered to be of a cylindrical shape
- The jacket temperature for heating in step 1 will be 120°C
- The jacket temperature for heating in Step 2 will be 210°C
- The density and specific heat value of Step 1 is 1.1 and 1.97, respectively
- The density and specific heat value of Step 2 is 1.03 and 1.81, respectively

The following calculations were done to determine the energy balance:

1. Height of the liquid mixture in the reactor (H, liq)

If the reactor is considered a cylinder, its volume can be approximated as
$V = \square*(D^2)/4*H$
Therefore, H, liq = [V, liq*4]/[$\square$*(D,reactor^2) and D,reactor = [(4*V,reactor)/(3*$\square$)]$^{1/3}$

2. Heat transfer area (A,h)

The heat transfer area is the surface area of the reactor, which can be approximated by a cylinder, such as
A,h = $\square$*D,reactor*H,fill + $\square$*(D,reactor^2)/4

3. Time required to heat the reaction mixture from room temperature to the desired temperature. This formula is also used to calculate the time required to cool the reaction mixture.

The heating time, in seconds, can be determined by the formula
t,heating = ln[(T,surr - T,final)/{T,surr - T,initial)]*(p,mix*V,reactor*C,p,mixture)/(U*A,h)

Normally, the reaction mixture would start at 25°C (i.e. room temperature). However, in step 1 of the process, the 3-pentadecylphenol is not added to the reaction mixture at room temperature. Because it is added the mixture at 55°C, this increases the reaction mixture to from 25°C to 30.7°C.

Table A14: Summary of the full energy balance around the jacketed reactor, R-201

Parameter	Step 1 Value	Step 2 Value
Starting Temperature	30.7°C	25°C
Final Temperature Required	90°C	180°C
Inlet Temperature in Heat Jacket	120°C	210°C
Height of Liquid Mixture	3.23 m	3.01 m
Heat Transfer Area	16.38 m^2	15.17 m^2
Time Required to Heat Reaction	43 min	75 min

Mixture		
Final Temperature of Reactants	80°C	80°C
Cooling Temperature of Heat Jacket	50°C	50°C
Time Required to Cool	11 min	60 min

Appendix L - Cycle Time Calculations

To determine the cycle time per batch to produce both the adduct as a result of step 1 and the final product as a result of step 2, the following assumptions were made:

- Assume that purging, charging, and sealing the reactor will take 2 hours
- Assume that any real times for physical processes (i.e.heating, cooling, and draining the reactor) are equivalent to 130% of the theoretical heating time
- Assume the outlet drain of the reactor has an inner pipe diameter of 2 inches
- Assume a height to diameter reactor ratio of 3:1
- The reactor is filled to 75% capacity in step 1 of the process
- The reactor is filled to 70% capacity in step 2 of the process
- Assume quenching will take 1 hour
- Assume all slurry processes will take 3 hours per slurry
- Assume that the process requires 2 slurries to reach a neutral pH in step 1
- Assume that the drying process will take 48 hours, based on the patent times [A2]

When calculating the cycle times to produce the adduct and final product, the steps used are shown below:

1. Time required to charge, seal and purge the reactor is assumed as 2 hours
2. Time required to heat the reaction mixture from room temperature to the desired temperature - refer to Appendix K
3. Time required to react the mixture in the reactor is dictated by the patent [A2]
4. Time required to drain the reaction mixture from the reactor

The draining time, in hours, can be determined by the formula

t,draining = [-A,cross sect. tank*2*(H.liq)^(½)] / [(2*g)^(½)*A.cross sect. outlet pipe)]

5. Time required for processes within the Nutsche filter are summarized below

Table A15: Summary of Nutsche filtering times for steps 1 and 2

Process	Time Required - Step 1	Time Required - Step 2
Quenching	1 hour	N/A
Filtering	N/A	1 hour
Slurrying	7 slurries * 3 hrs/slurry = 21 hours	4 slurries * 3 hrs/slurry = 12 hours
Drying	48 hours	48 hours
Total	70 hours	61 hours

Table A16: Summary of total reaction times for steps 1 & 2

Process	Time Required - Step 1	Time Required - Step 2
Charging, Sealing, Purging	2 hour	2 hours

Heating Time	1 hour	2 hours
Reaction time	3 hours	6 hours
Cooling Time	0.5 hour	1.5 hours
Draining Time	0.5 hour	0.5 hours
Nutsche Filter Times	70 hours	61 hours
Total	**77 hours**	**74 hours**

To compare the benefits of integrating 1, 2, or 3 Nutsche filters in our design, the team developed a diagram that illustrates the cycle times if these filters were run in parallel. Figure 6 helped to determine that 2 Nutsche filters reduced the average cycle time drastically, making it the optimal choice.

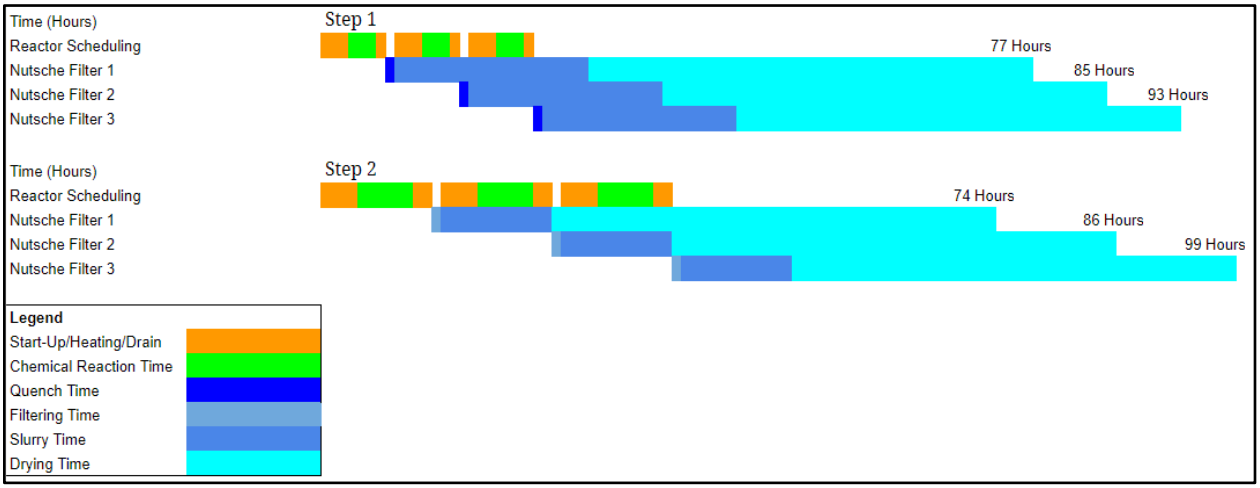


Figure A6: Visual depiction of parallel timing of the Nutsche Filters

Table A17: Cycle times dependent on the # of Nutsche filters available for Steps 1 & 2

Nutsche Filters in Design	Average Cycle Time Step 1	Average Cycle Time Step 2
1	77 hours	74 hours
2	42.5 hours	43 hours
3	31 hours	33 hours

Table A18: Sensitivity analysis around the delivery schedule and storage tank sizes

Storage Tank	Reagent Stored	8 Wk. Sched. Size (US gallons)	4 Wk. Sched. Size (US gallons)	2 Wk. Sched. Size (US gallons)	1 Wk. Sched. Size (US gallons)
Outdoor storage tank 1	NMP	56,700	28,400	14,200	7,100
Outdoor storage tank 2	DMSO	28,000	14,000	7,000	4,500
Outdoor storage tank 3	DMAE	1,300	700	400	200
Outdoor storage tank 4 -6	Methanol	123,100	61,600	30,800	*5200/batch
Outdoor storage tank 7	MEK	21,600	10,800	5,400	2,700
Outdoor storage tank 8	HCl	73,900	37,000	18,500	9,300
Outdoor storage tank 9	Toluene	4,000	4,000	4,000	5,000
Deionized water storage tank	Water	184,600	92,300	46,200	23,100
Hopper	4NPN *size limiting reagents	2200	1100	600	300
	K2CO3 anhydrous	1100	600	300	200
	Copper (II) acetate	500	300	200	100
Product storage tank 1	Adduct	7900	7900	7900	7900
Product storage tank 2	MPc	7900	7900	7900	7900

Appendix M - Process Flow Diagram for Step 1

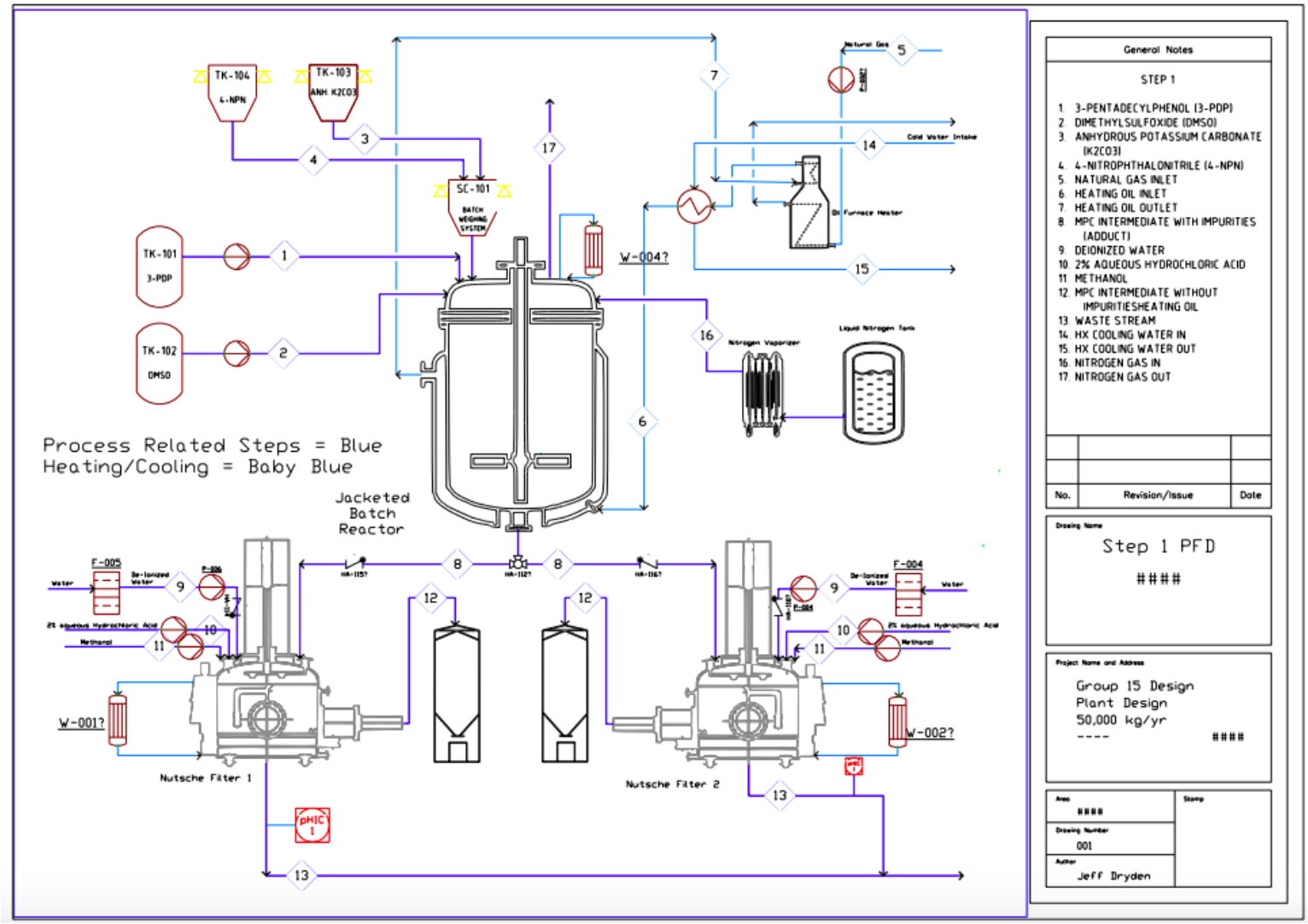


Figure A7: The process flow diagram for step 1 of the reaction, producing 1111 kg of adduct

Appendix N - Process Flow Diagram for Step 2

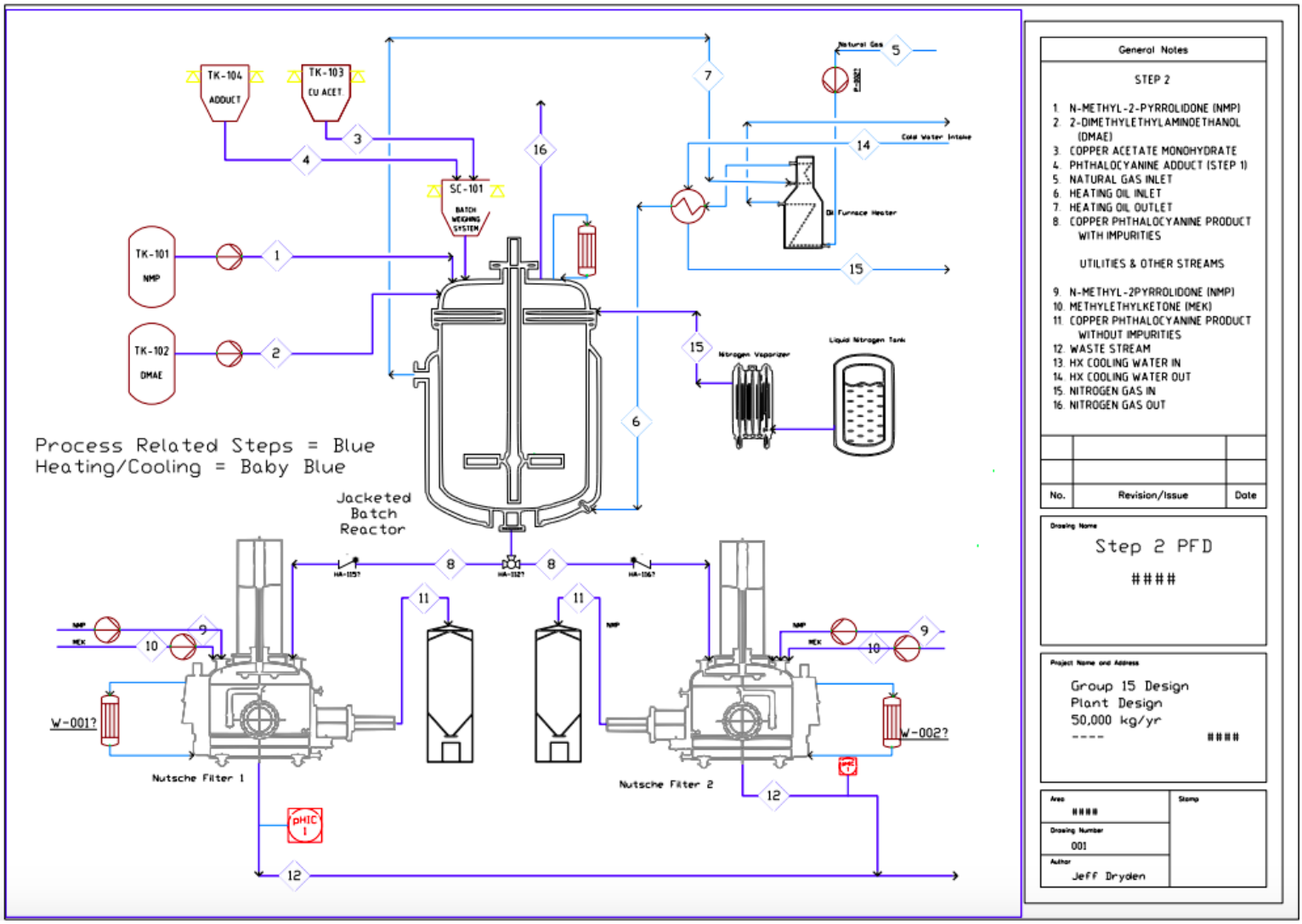


Figure A8: The process flow diagram for step 2 of the reaction, producing 803 kg of MPc

Appendix O - Equipment List

Table A19: Summary of all major equipment in the plant, except pumps (refer to Appendix P)

Equipment Type	Equipment Description	Electrical Classification	Equipment #	Material	Size (US gallons)	Equipment Cost (CAD)	Sources
Jacketed batch reactor	To house the charging, sealing, heating, reaction, cooling and draining of adduct/product	Class I, Group D, Division II	R-201	SS, 316	1,900	$402,416.71	[A25]
Nutsche filter 1	To house the charging, quenching, slurry, separation, drying and removing of adduct/product	Class I, Group D, Division II + Class II, Group E, Division II	N-101	Glass-steel filter	4,166	$950,000.00	[A26] Refer to appendix AI
Nutsche filter 2	To house the charging, quenching, slurry, separation, drying and removing of adduct/product	Class I, Group D, Division II + Class II, Group E, Division II	N-102	Glass-steel filter	4,166	$950,000.00	[A26] Refer to appendix AI
Hopper 1	To house the 4-NPN during stage 1 production, and copper (II) acetate during stage 2 production	Class II, Group E, Division I	T-301	SS, 316	300	$6,661.34	Refer to appendix AI
Hopper 2	To house the K2CO3 during stage 1 production, and the adduct during stage 2 production	Class II, Group E, Division I	T-302	SS, 316	300	$6,661.34	Refer to appendix AI
Weighted scale	To weigh the solids before discharging it into the reactor	Class II, Group E, Division II	T-201	SS, 316	*max weight 500 kg	$18,000.00	Refer to appendix AI
Furnace heater (preheater)	To heat the thermal fluid	Class I, Group D, Division I	H-201	SS, 316	*1.5 M BTU/hr	$54,498.64	[A27]
Heat exchangers	To cool the thermal fluid	Class I, Group D, Division I	H-202	Combination of carbon steel, stainless steel and iron	*64 m2 (688.89 ft2)	$40,281.60	[A27]
Condenser 1	To condense CH4 vapors from the drying process from Nutsche filter 1. This is a waste stream. We will use air cooled condensers, as the load (CH4 + MEK vapors) is relatively small	Class I, Group D, Division II	C-101	Copper-nickel air cooled condenser	*122 m2	$134,787.18	[A28, A29]

Condenser 2	To condense CH4 vapors from the drying process from Nutsche filter 2. This is a waste stream. We will use air cooled condensers, as the load (CH4 + MEK vapors) is relatively small	Class I, Group D, Division II	C-102	Copper-nickel air cooled condenser	*122 m2	$134,787.18	[A28, A29]
Condenser 3	To condense any vapors (i.e. mainly solvent) from the jacketed reactor and reflux them back into the reactor. Also to be used during the cleaning of the reactor.	Class I, Group D, Division II	C-201	Copper-nickel air cooled condenser	7.1 m2	$46,000.00	[A28, A29]
Deionizing filter	To deionize municipal water for process. Located in the Utilities Centre.	Class I, Group D, Division II	F-101	Fiberglass Dual Bed tank	2.4 m2	$13, 032.28	[A27, A30]
Product storage tank 1	To store the adduct/product after QA/QC. Located in the product storage warehouse.	Class II, Group E, Division I	T-101	SS, 316	7,900	$47,409.44	Refer to appendix AI
Product storage tank 2	To store the adduct/product after QA/QC. Located in the product storage warehouse.	Class II, Group E, Division I	T-102	SS, 316	7,900	$47,409.44	Refer to appendix AI
Outdoor storage tank 1	To store liquid NMP. Located in the tankfarm.	Class I, Group D, Division I	T-001	SS, 316	7,100	$44,467.59	Refer to appendix AI
Outdoor storage tank 2	To store liquid DMSO. Located in the tankfarm.	Class I, Group D, Division I	T-002	SS, 316	3,500	$29,089.04	Refer to appendix AI
Outdoor storage tank 3	To store liquid DMAE. Located in the tankfarm.	Class I, Group D, Division I	T-003	SS, 316	200	$5,222.84	Refer to appendix AI
Outdoor storage tank 4	To store liquid methanol. Located in the tankfarm.	Class I, Group D, Division I	T-004	SS, 316	5,200	$36,888.47	Refer to appendix AI
Outdoor storage tank 5	To store liquid methanol. Located in the tankfarm.	Class I, Group D, Division I	T-005	SS, 316	5,200	$36,888.47	Refer to appendix AI
Outdoor storage tank 6	To store liquid methanol. Located in the tankfarm.	Class I, Group D, Division I	T-006	SS, 316	5,200	$36,888.47	Refer to appendix AI
Outdoor storage tank 7	To store liquid MEK. Located in the tankfarm.	Class I, Group D, Division I	T-007	SS, 316	2,700	$24,894.70	Refer to appendix AI
Outdoor storage tank 8	To store concentrated HCl, and dilute it from 37% to 2%. Located in the tankfarm.	Class I, Group D, Division I	T-008	Corrosion-resistant polypropylene	700	$11,075.09	Refer to appendix AI
Outdoor storage tank 9	To store toluene for cleaning purposes. Located in the tankfarm.	Class I, Group D, Division I	T-009	SS, 316	5,000	$36,030.53	Refer to appendix AI

Nitrogen dewar	To store liquid nitrogen. Located separate from the tank farm, under a protected bank.	Class I, Group D, Division I	T-009	Cryogenic storage dewar tank	61	*$223/week	Refer to appendix AI
Nitrogen dewar	To store liquid nitrogen. Located separate from the tank farm, under a protected bank.	Class I, Group D, Division I	T-010	Cryogenic storage dewar tank	61	*$223/week	Refer to appendix AI
Nitrogen dewar	To store liquid nitrogen. Located separate from the tank farm, under a protected bank.	Class I, Group D, Division I	T-011	Cryogenic storage dewar tank	61	*$223/week	Refer to appendix AI
Nitrogen dewar	To store liquid nitrogen. Located separate from the tank farm, under a protected bank.	Class I, Group D, Division I	T-012	Cryogenic storage dewar tank	61	*$223/week	Refer to appendix AI
Bridge crane hoist	To lift and dispense large bulk solids. Located in the solids dispensing area.	Class II, Group D, Division II	C-101	/	/	$2,375.00	[A31]
Onsite transport truck	To have for onsite transportation purposes	Class II, Group D, Division II	TT-001	/	/	$207,900.00	[A32]
Fully powered stacker/forklift	To move products from shipping/receiving docks within the plant and product warehouse.	Class II, Group D, Division II	S-101	/	*load capacity of 2200 lbs	$8,200.00	[A33]
Fully powered stacker/forklift	To move products from shipping/receiving docks within the plant and product warehouse.	Class II, Group D, Division II	S-102	/	*load capacity of 2200 lbs	$8,200.00	[A33]
IBC Tote 1	To drain the reactor in the case of a faulty batch	Class I, Group D, Division II	I-101	Chemical-resistant HDPE	330	$657.00	[A34]
IBC Tote 2	To drain the Nutsche filter in the case of a faulty batch	Class I, Group D, Division II	I-102	Chemical-resistant HDPE	330	$657.00	[A34]
IBC Tote 3	To drain the Nutsche filter in the case of a faulty batch	Class I, Group D, Division II	I-103	Chemical-resistant HDPE	330	$657.00	[A34]
IBC Tote 4	To drain the Nutsche filter in the case of a faulty batch	Class I, Group D, Division II	I-104	Chemical-resistant HDPE	330	$657.00	[A34]
IBC Tote 5	To drain the Nutsche filter in the case of a faulty batch	Class I, Group D, Division II	I-105	Chemical-resistant HDPE	330	$657.00	[A34]
IBC Tote 6	To drain the Nutsche filter in the case of a faulty batch	Class I, Group D, Division II	I-106	Chemical-resistant	330	$657.00	[A34]

				HDPE			

Sample calculation of furnace heater (i.e. H-201):

To calculate the furnace heater capacity, the maximum heating requirements were analyzed. For this plant, this occurs during the heating of the reactor for step 2.

- Total energy required to heat the Reaction mixture to 180°C
  - Energy = Mass of Mixture * Specific Heat Capacity * Temperature Dif.
  - Energy = 5005kg * 1.918 kJ/kg*K * (180-25)°C
  - Energy = 1,400,824 kJ
- Total amount of time that heating takes place over
  - Heating takes place over 4,696 seconds
- Divide energy by time, and convert to BTU/hr
  - 1,400,824 kJ/4,696 seconds = 298 kW
  - 1,016,818 BTU/hr
- Assume Furnace is operating at 70% of maximum capacity
  - Capacity = 1,016,818 BTU/hr / 0.7
  - Capacity = 1,452,957 BTU/hr

Sample calculation of condenser around the Nutsche filters (i.e. C-101/C-102):

The following assumptions were made to calculate the sizing of C-101/C-102:

- Assme a 1:1 ratio between the surface area of the wet cake and the condenser
- Assume the Nutsche filter is filled to 85%, as the fill factor is between 75% and 85% for steps 1 and 2 of the process
- Assume the radius of the Nutsche filter is 1.85 m [A26]
- Assume the internal height of the Nutsche filter is 1.8 m [A26]

The surface area of the wet cake is equal to SA, wet cake = SA, condenser

$= 2*\square*R^2 + 2*\square*R*H$

$= 2*\square*(1.85)^2 + 2*\square*(1.85)*(1.80)$

$= 42.42\ m^2$

Sample calculation of storage tank (i.e. T-001):

1) Using the scale up factor and patented volumes required, calculate the volume of NMP required:

- Volume from patent = 315ml
- Scale up factor = 22697.36842
- Volume after scale up = 7149.67 L = $7.15m^3$

2) Using a fill factor of 80%, the volume of a cylindrical tank is given by $V= \square*R^2 * H$, such that H = 3D and R=D/:

- Therefore, V=□*D^2/4*3D and D=[(4*V)/ (FF*□*3)]$^{1/3}$
- Solving for the diameter of the tank, D=[(4*21.44901316m3)/(□*3*0.8)]^{⅓} = 2.25 m
- Solving the height of the tank, H=D*3 = 6.75 m
- Solving for the volume of the tank, V = □*D^2/4*H
  =□*2.25 m^2/4*6.75 m
  = 26.81 m^3

3) Converting the volume of the tank from m^3 to US gallons ($1m^3$ = 264.172 US gallons):

- V = 26.81 m^3 * 264.172 US gallons/m^3 = 7082.79 US gallons = 7100 US gallons

Appendix P - Pump Equipment List

The following are a list of assumptions that were used in pump sizing and costing calculations:

- Pumps were costed using the ChemEcon Queens software [A35]
- All pumps were costed for a material of stainless steel
- For friction losses, the estimated length of pipe multiplied by a factor of 4 to account for bends and elbows
- Pipe pressure loss is calculated based on pipe diameter
- Flow elements result in 3 psi pressure loss
- Control valves result in 10 psi pressure loss

1. Determine the flow
   Normal flow rate was selected, and rated flow rate was calculated:
   $$Rated\ Flow = \frac{Normal\ Flow\ \times\ 1.2}{(1 - 0.15)}$$

2. Piping friction losses
   $$piping\ friction\ losses\ =\ estimated\ length\ of\ pipe \times 4 \times pipe\ pressure\ loss$$

3. Determine pump inlet pressure
   $$Suction\ Pressure = source\ tank\ pressure - piping\ friction\ losses \pm static\ head$$

4. Determine pump discharge pressure
   $$Discharge\ Pressure = destination\ pressure + piping\ friction\ loss + control\ valve\ losses \pm static\ head + equipment\ losses$$

5. Calculate shaft power (HP)
   $$Power\ = \frac{rated\ flow\ \times\ differential\ pressure}{1714\ \times\ efficiency}$$

Table A20: Summary of all major pumps used in the plant

Equipment Type	Equipment Description	Equipment Classification	Equipment #	Material	Power (kW)	Normal Discharge Pressure (Bar g)	Pump Suction Pipe Size	Pump Discharge Pipe Size	Equipment Cost (CAD)
Filter 1 Pump 1	Centrifugal pump to move deionized water to N-101	Class I, Group D, Division II	P-101	SS, 316	1.44	1.85	4	3.5	$8,564.16 [A35]
Filter 1 Pump 2	Centrifugal pump to move HCl to N-101	Class I, Group D, Division I	P-102	Polypropylene	3.59	2.9	3.5	3	$9,942.55 [A35]
Filter 1 Pump 3	Centrifugal pump to move methanol to N-101	Class I, Group D, Division I	P-103	SS, 316	3.74	2.32	5	4	$10,035.24 [A35]
Filter 1 Pump 4	Centrifugal pump to move NMP to N-101	Class I, Group D, Division I	P-104	SS, 316	1.31	2.73	2.5	2	$8,487.26 [A35]
Filter 1 Pump 5	Centrifugal pump to move MEK to N-101	Class I, Group D, Division I	P-105	SS, 316	3.29	2.31	5	4	$9,755.22 [A35]
Filter 2 Pump 7	Centrifugal pump to move deionized water to N-102	Class I, Group D, Division II	P-106	SS, 316	1.44	1.85	4	3.5	$8,564.16 [A35]
Filter 2 Pump 8	Centrifugal pump to move HCl to N-102	Class I, Group D, Division I	P-107	SS, 316	3.59	2.9	3.5	3	$9,942.55 [A35]
Filter 2 Pump 9	Centrifugal pump to move methanol to N-102	Class I, Group D, Division I	P-108	SS, 316	3.74	2.32	5	4	$10,035.24 [A35]
Filter 2 Pump 10	Centrifugal pump to move NMP to N-102	Class I, Group D, Division I	P-109	SS, 316	1.31	2.73	2.5	2	$8,487.26 [A35]
Filter 2 Pump 11	Centrifugal pump to move MEK to N-102	Class I, Group D, Division I	P-110	SS, 316	3.29	2.31	5	4	$9,755.22 [A35]

Reactor Pump 1	Positive displacement pump to move 3-PDP into reactor	Class I, Group D, Division I	P-201	SS, 316	1.47	3.91	2	1.5	$12,689.48 [A35]
Reactor Pump 2	Centrifugal pump to move DMSO into reactor	Class I, Group D, Division I	P-202	SS, 316	2.52	3.85	2.5	2	$9,261.25 [A35]
Reactor Pump 3	Centrifugal pump to move NMP into reactor	Class I, Group D, Division I	P-203	SS, 316	2.36	3.66	2.5	2	$9,156.73 [A35]
Reactor Pump 4	Reciprocating pump to move DMAE into reactor	Class I, Group D, Division I	P-204	SS, 316	0.72	4.83	1.25	1	$23,511.52 [A35]
Reactor Pump 5	Centrifugal pump to move toluene into reactor	Class I, Group D, Division I	P-205	SS, 316	2.41	3.67	2.5	2	$9,189.27 [A35]

Appendix Q - Key Unit Piping and Instrumentation Diagram (P&ID)

The P&ID below depicts the first step of the process, which produces the MPc adduct. The P&ID for step 2 is very similar. Most of the same equipment is used, with the main difference being the reactants/solvents that enter the reactor. See the note in the figure below for the stream compositions in the step 2 process.

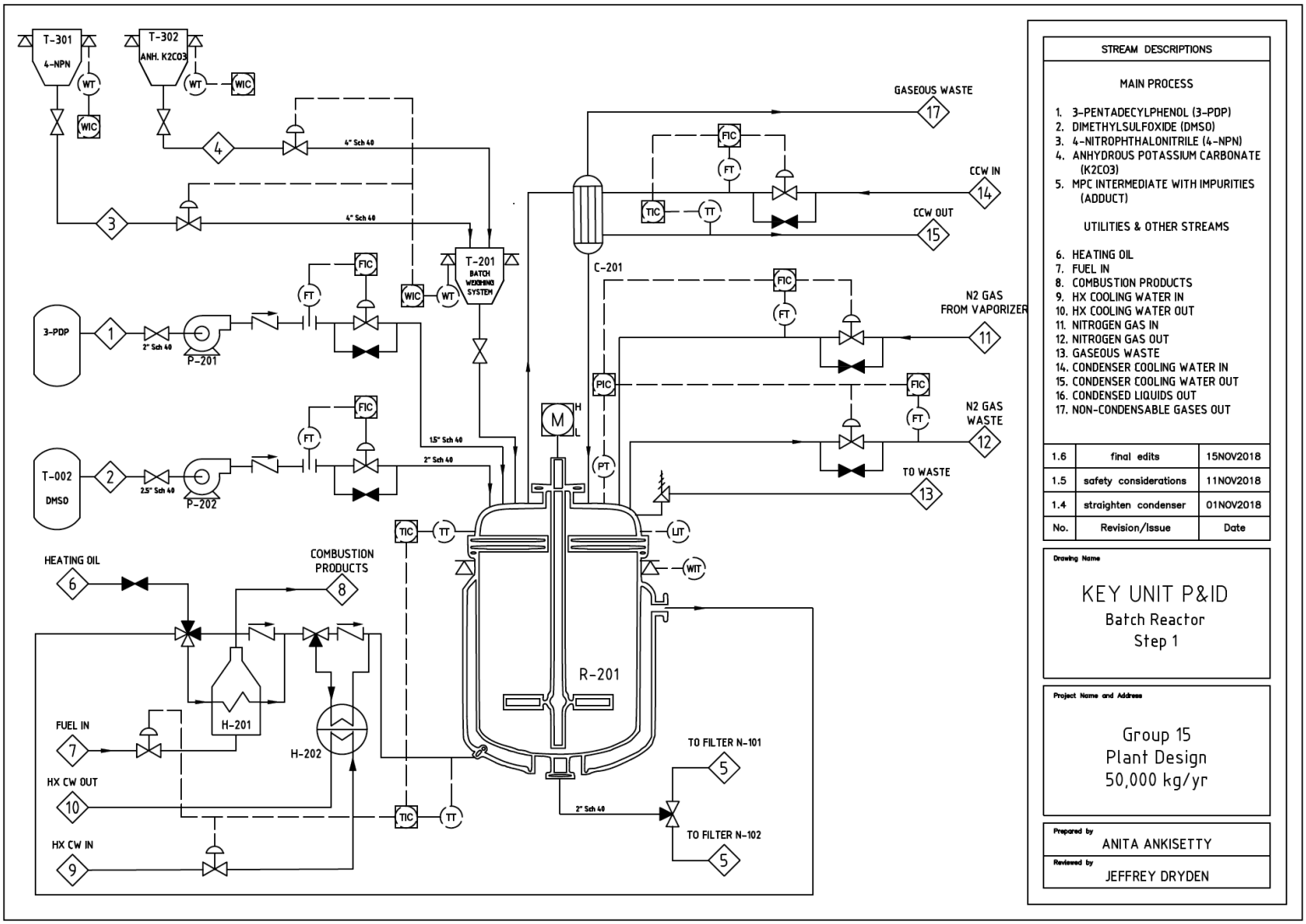


Figure A9: Key unit P&ID for jacketed reactor as used in step 1, to produce the MPc adduct

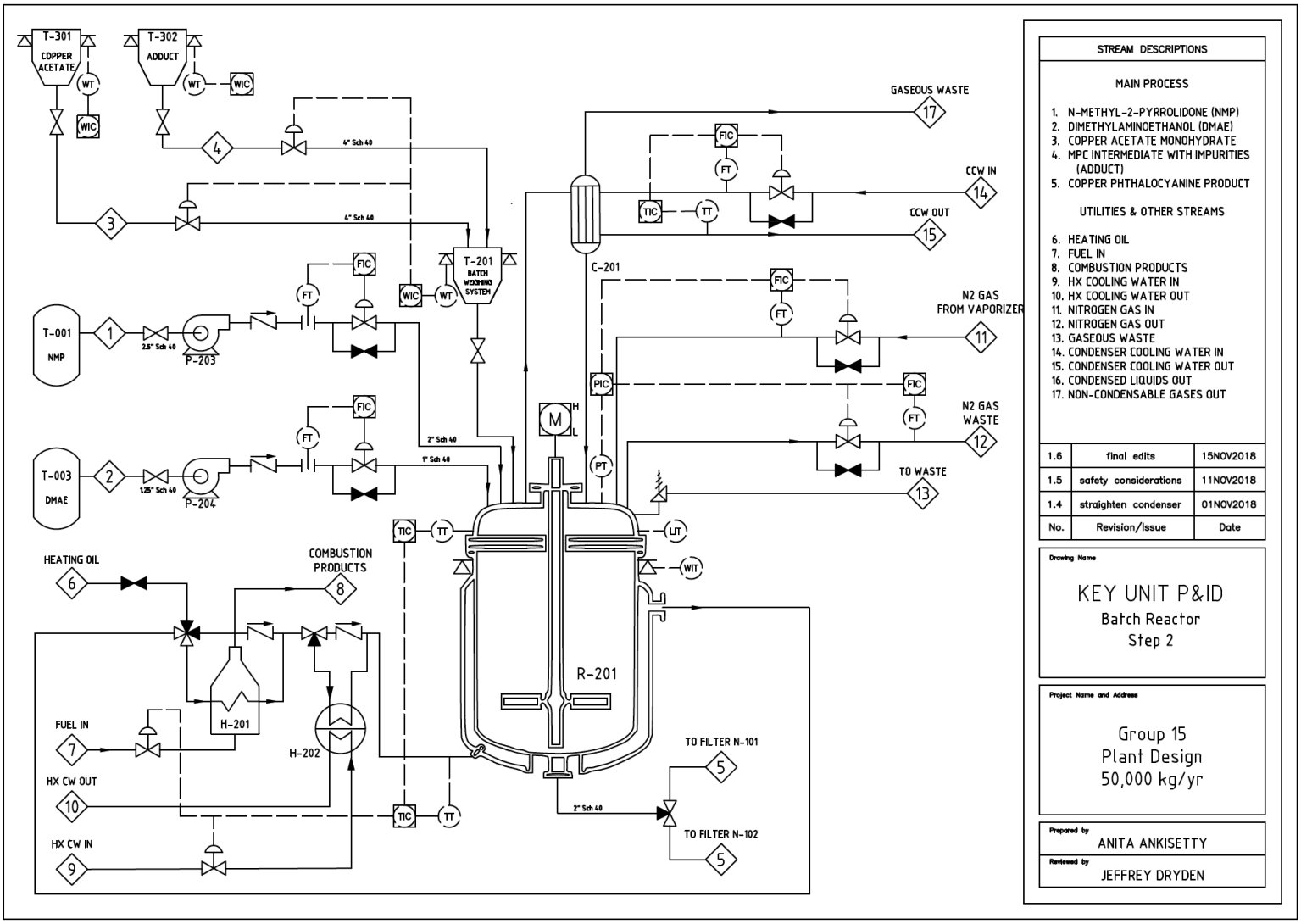


Figure A10: Key unit P&ID for jacketed reactor as used in step 2, to produce the final product

Appendix R - Top View of Reactor

As Figure 11 illustrates below, the 6" port is for charging the chemical reactants into the reactor, the 4" ports are for instrumentation and the viewing port, while the 12" flange is for the condenser.

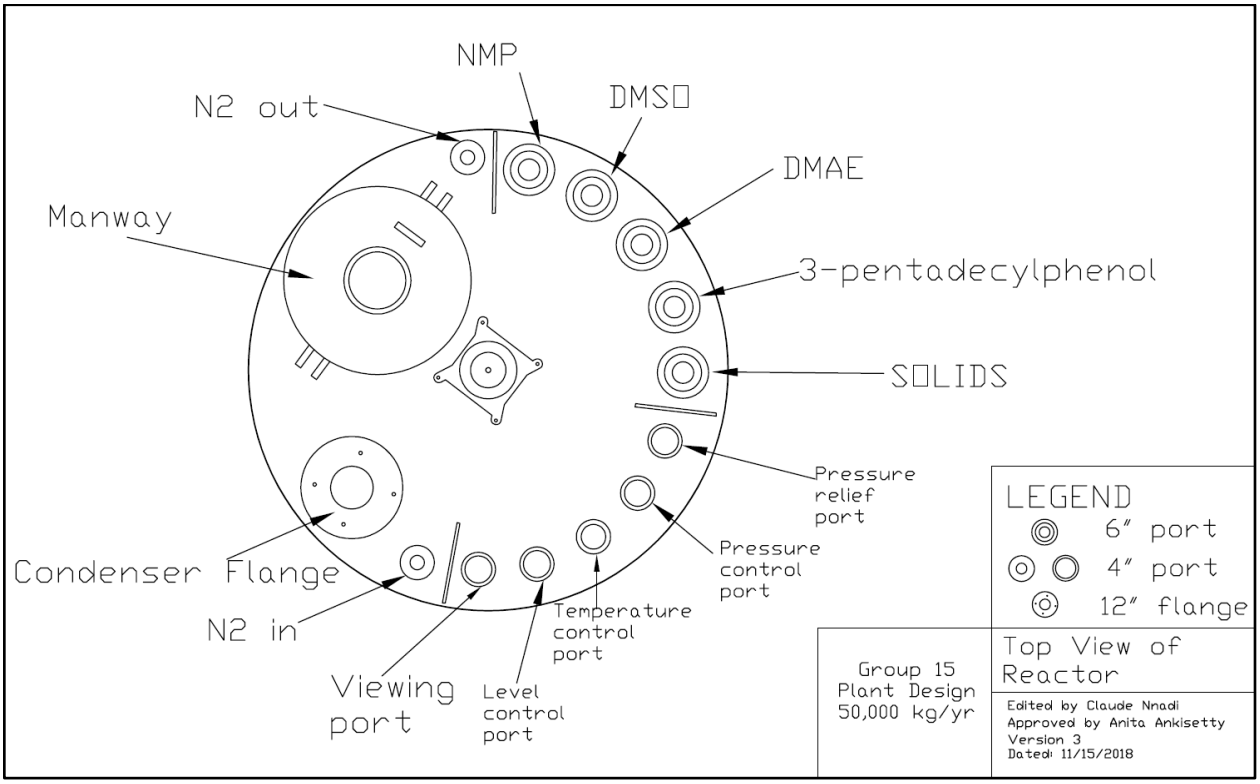


Figure A11: 2D drawing of the top of the jacketed batch reactor

Appendix S - Site Layout

Located off of Highway 40 and Indian Road South, the plant perimeters are indicated by the thick black line. The complete site is encompassed by an area of 0.02 km^2, with site-wide dimensions of 150 m by 140 m. All non-production and non-operational buildings are 6 m apart, and all other dimensions are indicated on figure 12. The areas marked as "expandable areas" provide the client with flexible spaces to expand future operations.

Figure A12: A detailed 2D site layout of the proposed chemical plant

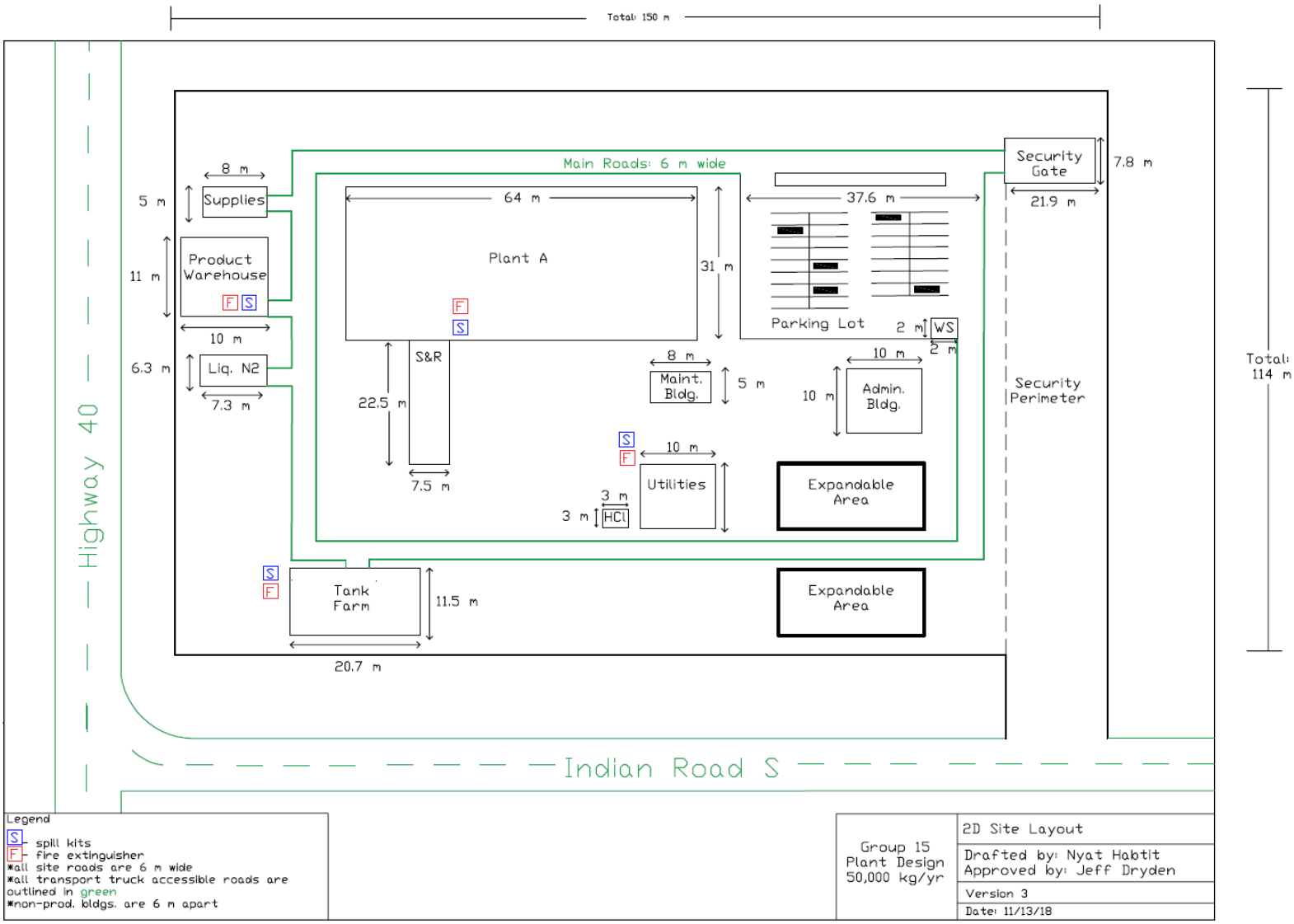


Table A21: Summary of Site Layout [A36]

Site Area	Function	Length (m)	Width (m)
Plant A	Produces adduct and MPcs	31	64
Shipping and Receiving (S&R) Docks	Able to ship final product, receive bulk solids and accept large equipment.	22.5	7.5
Supplies Centre	Stores PPE for personnel, spill kits, and additional safety measure tools.	5	8
Product Warehouse	Stores adduct and MPcs until it needs to be shipped to the customer.	11	10
Tank Farm	Stores all solvents and alcohols	11.5	20.7
HCl Storage	Stores concentrated (37%) HCl	3	3
Liquid Nitrogen Tank Storage	Stores four cryogenic liquid nitrogen tanks	6.3	7.3
Utilities Building	Main building to distribute natural gas, municipal water and thermal fluid	10	10
Maintenance Building	Space for maintenance team to store their equipment/tools, as well as backup equipment	5	8
Administrative Building	Office spaces	10	10
Parking Lot	Parking space for all personal vehicles	37.6	28

Appendix T - Transport Truck Pathway Layout

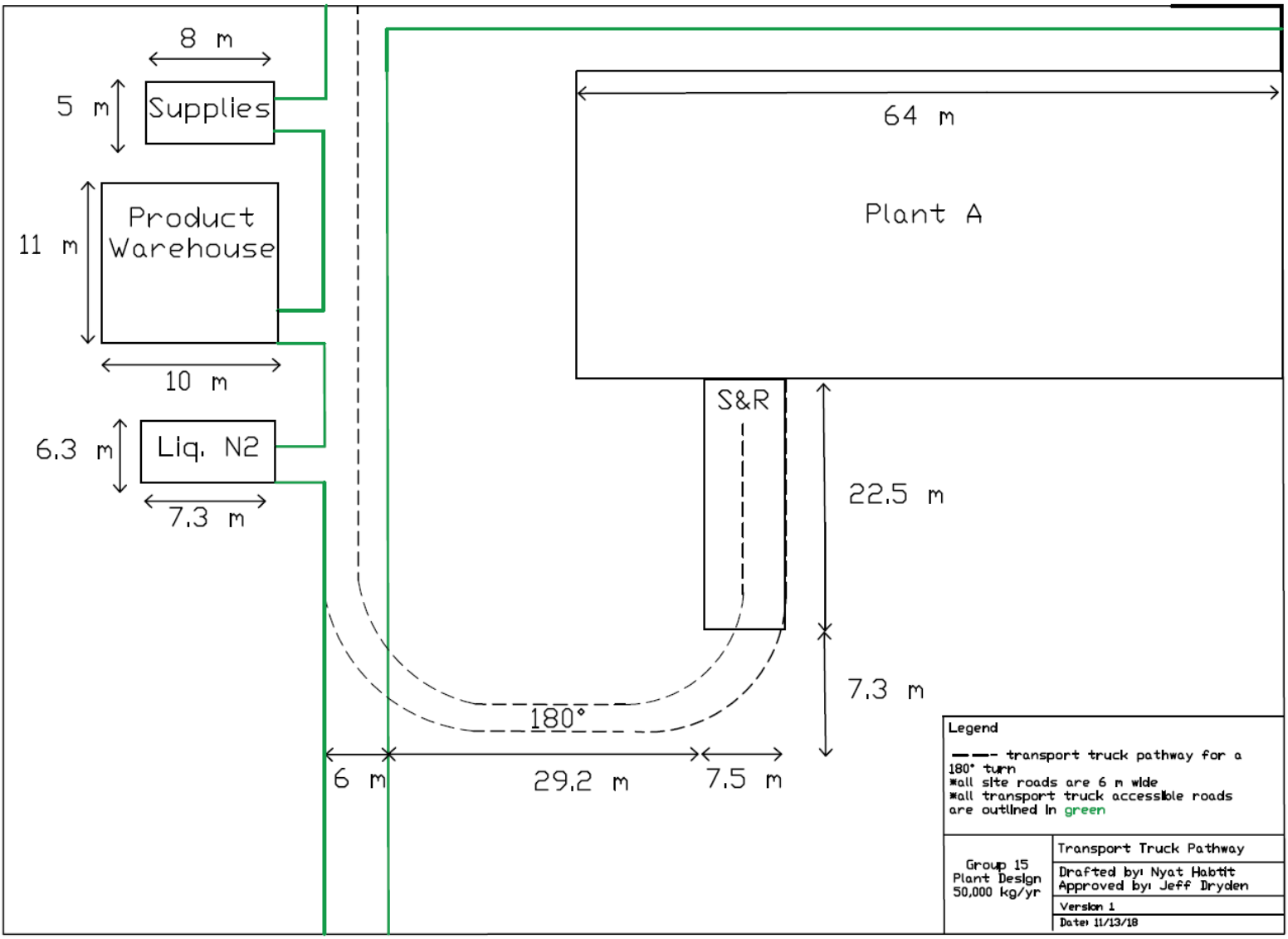


Figure A13: A 2D model of a transport trucks' turning radius

The following assumption were made to determine the truck's turning radius:

- An average transport truck is 14.6 m long [A37], 2.6 m wide
- Assume a turning radius of 180° requires a distance of two times the length of the vehicle

Therefore, transport trucks onsite will require a minimum distance of 29.2 m to turn 180° from the main road into the shipping and receiving docks.

Appendix U - 2D Horizontal Plant Layout

The overall plant is 31 m long and 64 m wide.

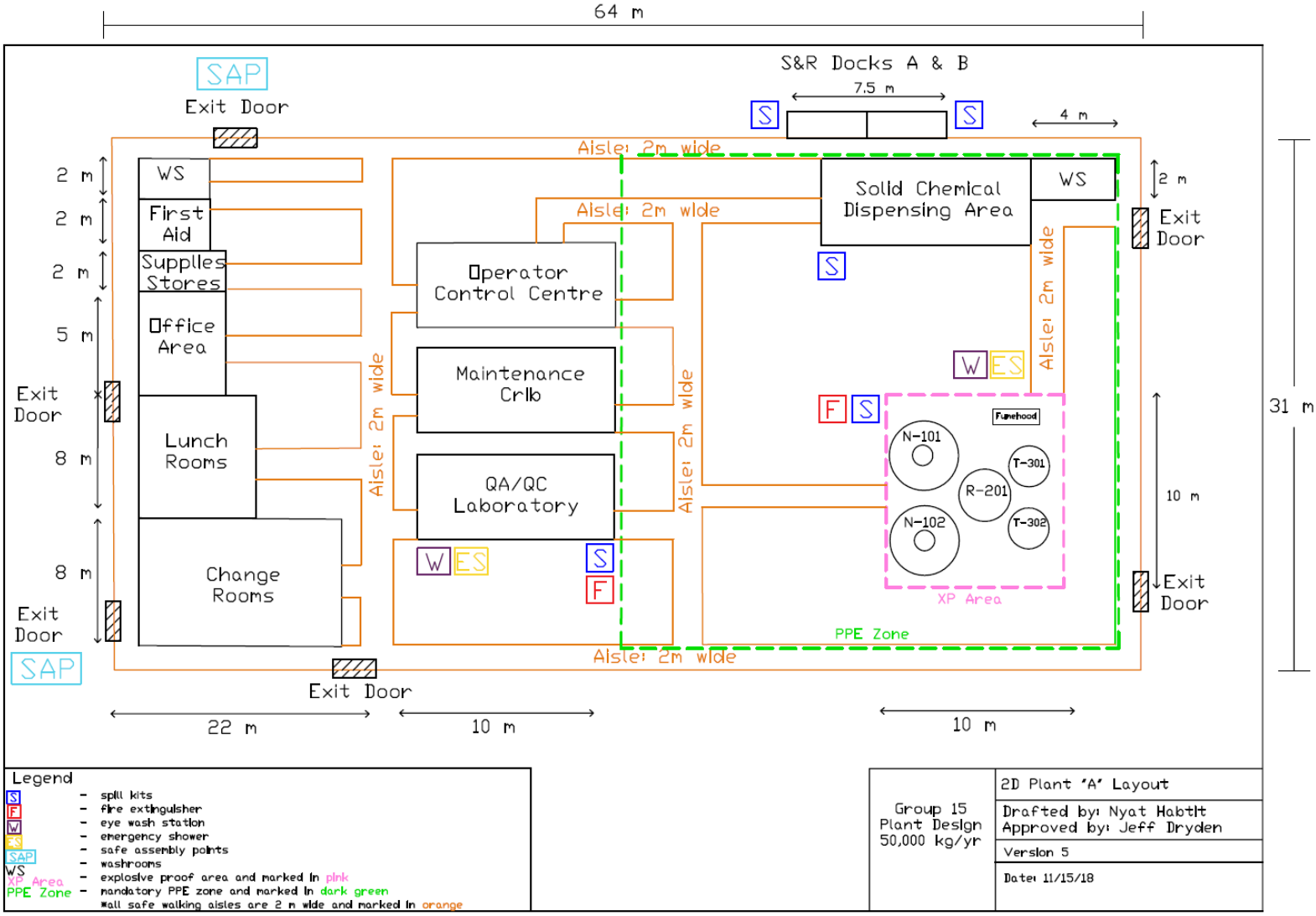


Figure A14: A detailed 2D plant layout of the Plant "A"

Table A22: Summary of Plant Layout [A36]

Plant Area	Function	Length (m)	Width (m)
Aisles	A safe walking aisle	/	2
Washrooms	For any plant personnel (x2)	2	4
First Aid Centre	For any non-emergency injuries	2	4

Supplies Stores	To store personnel PPE	2	6
Office Area	Office space plant management and administrators	5	6
Lunch Room	For recreational purposes (i.e. lunch, socializing)	8	10
Change Rooms	Includes lockers	8	22
Operator Control Centre	Control room for operators/technicians	6	10
Maintenance Crib	Onsite storage space for maintenance tools and equipment	5	10
QA/QC Laboratory	Laboratory to test purity of product	5	10
Shipping and Receiving Docks	Docks for transport trucks to unload/load	22.5	7.5
Solid Chemical Dispensing Area	Area for solids bulk handling	4	10
Explosion-proof Area	Production area with XP walls	10	10

Appendix V - 2D Vertical Plant Layout

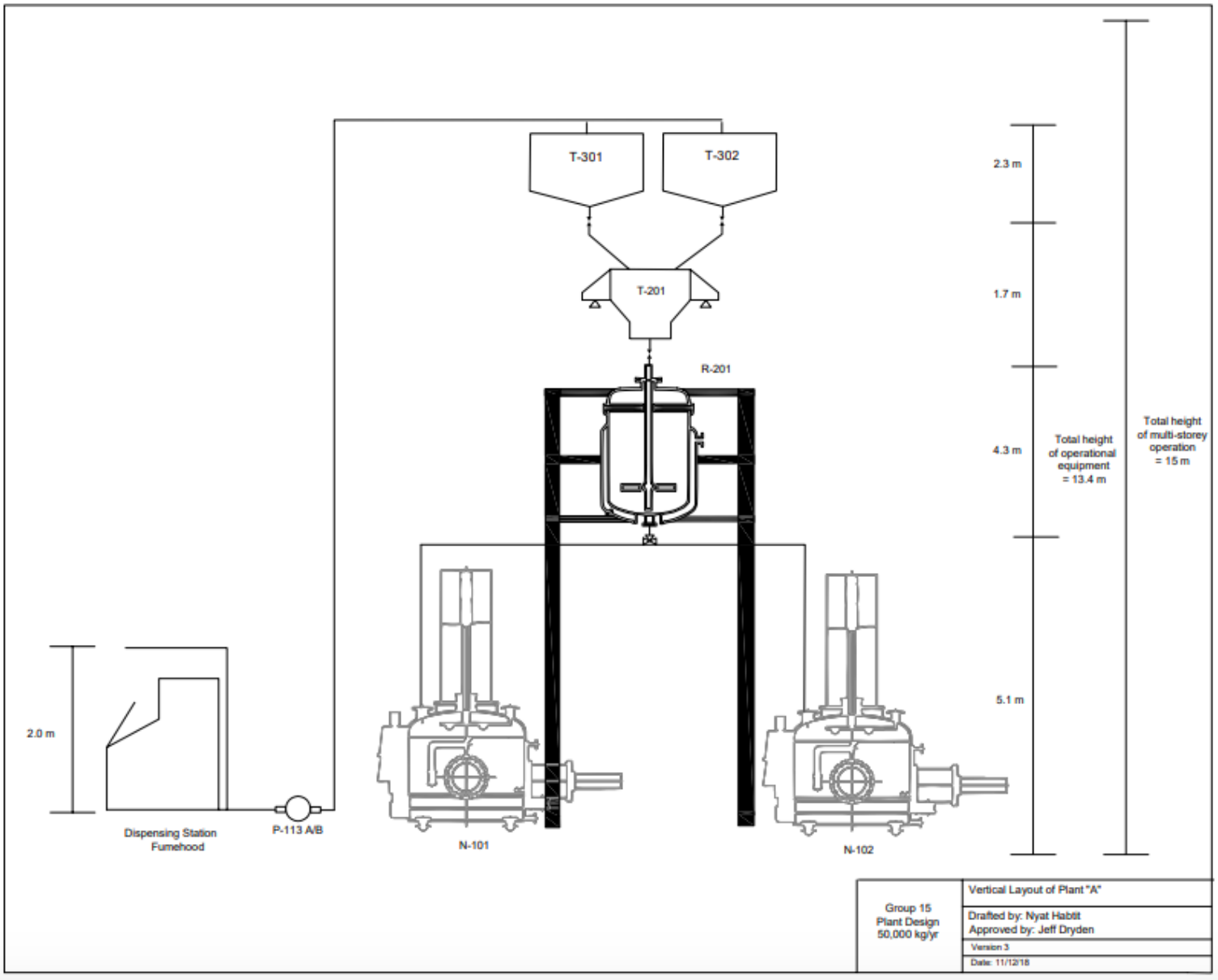
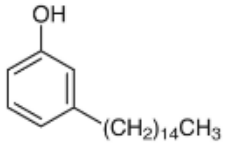
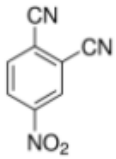
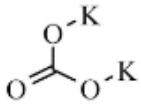


Figure A15: A vertical orientation of the multi-storey area of the plant

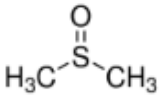
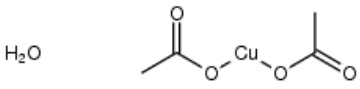
Appendix W - Safety Summary Sheet

Table A23: The safety summary sheet showing 3 reactants, 3-Pentadecylphenol, 4-Nitrophthalonitrile and Anhydrous Potassium Carbonate

Chemical	3-Pentadecylphenol	4-nitrophthalonitrile	Anhydrous Potassium Carbonate
Structure			
GHS Pictogram			
GHS Classification	Acute toxicity, Oral (category 4) Acute toxicity, Inhalation (category 4) Acute toxicity, Dermal (category 4) Skin corrosion/irritation (category 2) Serious eye damage/irritation (category 2A) Specific target organ toxicity - single exposure (category 3), respiratory system	Acute toxicity, Oral (category 4) Skin irritation (category 2) Eye irritation (category 2A) Specific target organ toxicity - single exposure (category 3)	Acute toxicity, Oral (category 4) Acute toxicity, Inhalation (category 4) Acute toxicity, Dermal (category 4) Skin corrosion/irritation (category 2) Serious eye damage/irritation (category 2A) Specific target organ toxicity - single exposure (category 3), respiratory system Acute hazard - Harmful to aquatic life (category 3)
Potential Health Effects	Inhalation: May cause respiratory tract irritation Skin: May cause skin irritation Eyes: May cause eye irritation Ingestion: Harmful if swallowed	Inhalation: May cause respiratory tract irritation Skin: Causes skin irritation Eyes: Causes eye irritation Ingestion: Harmful if swallowed	Inhalation: May cause respiratory tract irritation, harmful if inhaled Skin: Causes skin irritation Eyes: Causes eye irritation Ingestion: Harmful if swallowed
First aid Measures	General advice: Consult a physician, show the safety sheet to doctor and move out of the dangerous area	General advice: Consult a physician, show the safety sheet to doctor and move out of the dangerous area	--
Conditions of flammability	Not flammable or combustible	Not flammable or combustible	Not flammable or combustible
Handling	Avoid contact with skin and eyes. Avoid formation of dusts and aerosols. Provide appropriate exhaust ventilation at places	--	--

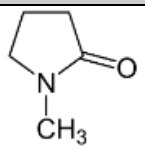
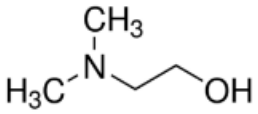
	where dust is formed		
Storage	Storage temperature of 2-8°C	Store in a dry, well-ventilated place	Store in a well-ventilated place
Exposure control	Respiratory: Type P95 or type P1 respirator Hand protection: Nitrile rubber gloves Eye protection: Safety glasses with side shields Skin and body protection: Chemical suit	Respiratory: Type P95 or type P1 respirator Hand protection: Gloves Eye protection: Safety glasses with side shields Skin and body protection: Chemical suit	Respiratory: A NIOSH approved respirator with N95 cartridges permissible when airborne concentrations are expected to exceed limits Hand: Appropriate chemical resistant gloves Eye protection: Safety glasses with side shields Skin and body protection: Protective clothing
Melting point	50-53°C	142-144°C	891°C
Boiling point	190-195°C	--	--
Flash point	113°C	--	Not Flammable
Chemical stability	Stable under recommended storage conditions	Stable under recommended storage conditions	Stable at normal temperatures and pressures

Table A24: Safety summary sheet showing DMSO, Nitrogen and Copper Acetate Monohydrate

Chemical	Dimethylsulfoxide	Nitrogen	Copper Acetate Monohydrate
Structure			
GHS Pictogram	N/A		
GHS Classification	Flammable liquids (category 4)	Simple asphyxiant Compressed gas	Acute toxicity, Oral (category 4) Skin corrosion/irritation (category 2) Serious eye damage/irritation (category 2A) Specific target organ toxicity - single exposure (cateogry 3), respiratory system

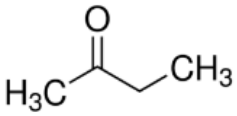
Potential Health Effects	--	--	Harmful if swallowed Causes skin irritation Causes serious eye irritation May cause respiratory irritation
First aid Measures	Consult a physician and show the SDS	Remove to fresh air, clear airways, give artificial respiration, call a physician	Do not induce vomiting if swallowed. Move to fresh air if inhaled. Call Physician. Wash off immediately with plenty of water in case of skin contact
Conditions of flammability	Flammable	Pressurized container may burst if heated	Non flammable
Handling	Avoid inhalation of vapor Keep away from sources of ignition	Wear leather safety gloves and safety shoes Protect cylinders from any form of physical damage	--
Storage	Store under inert gas, hygroscopic	Store in a cool, ventilated place. Temp less than 52°C	Store in a well ventilated area
Exposure control	Respiratory: A NIOSH approved respirator Hand: Nitrile rubber gloves Eye protection: Safety glasses with side shields Skin and body protection: Impervious clothing	Respiratory: A NIOSH approved respirator, respirable fume respirator or air supplied respirator Hand: Heavy rubber gloves Eye protection: Safety glasses with side shields Skin and body protection: Impervious clothing	Respiratory: Follow the OSHA respiratory guidelines Hand: Appropriate gloves Eye protection: Appropriate safety glasses Skin and body protection: Impervious clothing
Melting point	16-19°C	-210°C	115°C
Boiling point	189°C	-195.8°C	--
Flash point	87°C	--	--
Chemical stability	Stable under recommended storage conditions	Reacts violently with lithium, titanium, neodymium to form nitrides. Can also combine with hydrogen and oxygen at high temperatures	Stable under normal conditions

Table A25: Safety summary sheet showing HCl, NMP and DMAE

Chemical	Hydrochloric acid	NMP	2-dimethylaminoethanol
Structure	H−Cl		

GHS Pictogram			
GHS Classification	Corrosive to metals (category 1) Skin corrosion/irritation (category 1B) Serious eye damage (category 1) Specific target organ toxicity - single exposure (category 3), respiratory system	Flammable liquids (category 4) Eye irritation (category 2) Reproductive toxicity (category 1B) Specific target organ toxicity - single exposure (category 3), respiratory system	Flammable liquids (category 3) Acute toxicity, Oral (category 4) Acute toxicity, Inhalation (category 3) Acute toxicity, Dermal (category 4) Skin corrosion/irritation (category 1B) Serious eye damage (category 1) Acute aquatic toxicity (category 3)
Potential Health Effects	--	--	--
First aid Measures	Take off contaminated clothing If inhaled, provide fresh air When it comes in contact with eyes or skin, wash with water for at least 15 minutes	Consult physician, show safety sheet and clear the area	Take off contaminated clothing If inhaled, provide fresh air When it comes in contact with skin, rinse with water and soap
Conditions of flammability	Non flammable	Flammable	--
Handling	--	Avoid contact with eyes and skin. Do not inhale vapors and mist. Keep away from sources of ignition	Avoid contact with eyes and skin. Do not inhale vapors and mist. Keep away from sources of ignition
Storage	Store in corrosive resistant polypropylene	Store under inert gas, moisture sensitive	Store under inert gas
Exposure control	Respiratory: Follow the OSHA respiratory guidelines, use Type E acid gas filters Hand: Appropriate gloves Eye protection: Appropriate safety glasses Skin and body protection: Impervious clothing	Respiratory: Full face respirator with multi-purpose combinations Hand: Butyl rubber gloves Eye protection: Safety glasses with side shields Skin and body protection: Impervious clothing	Respiratory: Full face respirator with multi-purpose combinations Hand: Nitrile rubber gloves Eye protection: Tight fitting safety goggles Skin and body protection: Complete suit protecting against chemicals
Melting point	-35°C	-24°C	-70°C
Boiling point	57°C	202°C	134-136°C
Flash point	--	91°C	39°C
Chemical stability	Stable under normal conditions	Stable under recommended storage conditions	Stable under recommended storage conditions

Table A26: Safety sheet summary sheet showing MEK

Chemical	MEK
Structure	
GHS Pictogram	
GHS Classification	Highly flammable liquid and vapour Causes serious eye irritation
Potential Health Effects	--
First aid Measures	Take off contaminated clothing If inhaled, provide fresh air When it comes in contact with skin, rinse and use barrier cream
Conditions of flammability	Flammable, Vapours heavier than air so beware of reignition
Handling	Use an extractor Keep away from sources of ignition
Storage	Store in an area with temperature between 15-25°C
Exposure control	Respiratory: An approved respirator Hand: Butyl rubber gloves Eye protection: Safety glasses with side shields Skin and body protection: Impervious, flame retardant clothing
Melting point	-86°C
Boiling point	79-80°C
Flash point	-8°C
Chemical stability	Reactive if exposed to light and air

Appendix X - Process Safety Analysis

Table A27: Process Safety Analysis for the reactor and Nutsche filter

Guide Word	Deviation	Alarm/Indicator	Causes	Consequences	Actions
Analysis for Reactor					

None	No Agitation in reactor	Viewing port on the top of the reactor Sensor that measures RPM	Motor stops working	Operation interrupted: ●Production delay ●Purity of product reduces	●Call maintenance operators to service the motor ●Test the motor and agitator before every run
			Reactor content is too waxy (viscous)	Operation interrupted: ●Production Delay ●Yield percentage drops ●Purity of product reduces	Drain the reactor and wash before starting the reaction again
Less	Low temperature	Temperature indicator of reactor contents Temperature indicator of inlet heating fluid High and Low Temperature Alarm Level indicator and alarm in the reactor	Leaking pipe/jacket	Operation Interrupted: ●No reaction ●Fires can start in the insulation ●Production delay	●Fix the leaking pipe ●Use the proper material for the pipe to prevent corrosion, DOWTHERM Q heat transfer fluid is non-corrosive towards common metals and alloys
			Not enough fuel supplied to the furnace	Operation Interrupted: ●No reaction ●Production Delay	●Supply more fuel to the furnace ●Check that there are no leaks along the fuel supply line
			Too much cooling water supplied to the heat exchanger	Operation Interrupted: ●No reaction ●Production Delay ●Low product yield and purity	Reduce the cooling water flow
			Pump stops working	Operation Interrupted: ●No reaction ●Production Delay	●Automatic startup of the backup reactor ●Replace the pump
More	High temperature		Furnace temperature is high	Operation Interrupted: ●No reaction ●Production Delay ●Evaporation of solvents	●Reduce the furnace temperature ●Run reaction when the furnace is at the right temperature
			Heat exchanger not functioning	Operation Interrupted: ●No reaction /Side reactions ●Production Delay	●Use a backup heat exchanger ●Repair the malfunctioning heat exchanger
Less	Low pressure in the reactor	Pressure indicator for the reactor	Vacuum pump is turned on	Operation Interrupted: ●No reaction or off-spec product	●Wear appropriate PPE ●Check pipes for leaks frequently

More	More pressure in reactor	High and Low Pressure Alarm	Too much Nitrogen supplied to the reactor	Operation Interrupted: ●No reaction or off-spec product ●Possible reactor explosion due to high pressure	●PRV ruptures at fixed setpoint ●Regular maintenance and safety checks to make sure this doesn't happen
			Formation of CO2 during Step 1 of the reaction	Operation Interrupted: ●If pressure gets too high the PRV might rupture ●Nothing might happen	●PRV ruptures at fixed setpoint
More	More liquids in reactor (Solvents)	Level indicator and alarm in the reactor Flow rate indicator along the pipeline	Feed flowrate is increased	Operation Interrupted: ●Waste disposal required for wasted reactants ●Risk of overfilling the reactor	●Reduce the flow into the reactor ●Disposal of waste following required standards
Less	Less liquids in reactor (Solvents)		Old/malfunctioning pump	Operation Interrupted: ●Low product yield ●Production Delay ●Improper mixing	Maintenance required for pump, replace pump if required
			Leaking pipe/tank	Operation Interrupted: ●Low product yield ●Production Delay ●Liquid reactants exposed to surroundings/ environment	●Fix the leak ●Proper disposal of the reactants required
More	More Oxygen concentration in the reactor	Oxygen concentration sensor	Not enough inert gas supplied	Operation Interrupted: ●Side reactions could occur with oxygen ●Production Delay	Increase the flow of inert gas to inert reactor
Analysis for the filter					
More	More temperature in filter	Temperature indicator inside the filter	Not enough quenching water	Operation Interrupted: ●Low product yield ●Production Delay	Quench with more water
			Not enough cooling time	Operation Interrupted: ●Low product yield ●Production Delay	Let the mixture cool in the filter

Less	Low pH of the filtrate	pH Indicator on the waste stream	High HCl concentration	Operation Interrupted: ●Impure product ●Production Delay ●Acidic filtrate	Dilute the stream with a base or water to get to neutral pH
			Not enough slurries with water	Operation Interrupted: ●Impure product ●Production Delay	Keep reslurrying until the pH indicator shows neutral
More	More pressure during vacuum drying	Pressure indicator	Vacuum pump not working	Operation Interrupted: ●High moisture content in product ●Longer drying times	Maintenance required for pump, replace pump if required
None	No Agitation in filter	Viewing port	Motor stops working	Operation interrupted: ●Production delay ●Improper washing ●Low product purity	●Call maintenance operators to service the motor ●Test the motor and agitator before every run

Appendix Y - Hazard Analysis

Table A28: Risk Analysis for the entire chemical process

Hazard/Risk	Cause	Mitigation
Dangerous chemical reactions	Chemical incompatibility	Incompatible chemicals have seperate tank farms
Explosion	Nitrogen Gas	Nitrogen gas is kept in a different storage building, Buildings built with blast walls
Reprotoxicity	NMP	There is little to no contact with NMP as NMP goes from the storage tank to the batch reactor via pipes
Falls	Tripping on liquids, cables etc, falling from high levels	Guards such as rail guards will be installed to prevent falls
Injuries during maintenance	Equipment left running or not shut off properly	Proper Lockout/Tagout
Environmental Pollution	Spills and Leaks from the entire process (starting from the storage of the reactants to the storage of the product)	-Containment areas for the storage tanks, 110% of the volume of the largest tank in the tank farm -Spill kits -Monitors for CO_2

Appendix Z - Chemical Compatibility

Table A29: Table of Chemical compatibilities and solubilities

Chemicals	Incompatible in	Soluble in	What happens under flammable conditions
DMSO	Acid chlorides, strong acids, strong oxidizing and reducing agents, phosphorus halides	Alcohol and Diethyl ether	Produces sulfur dioxide
DMAE	Oxidizing agents, copper, zinc, iron, Do not store near acids	N/A	Produces nitrous oxides, carbon dioxides
NMP	Strong acids, strong oxidizing and reducing agents,	N/A	Produces nitrous oxides, carbon dioxides
HCl	Metals, strong oxidizing agents, bases, sodium hypochlorite, amines, fluorines, cyanides, alkaline	N/A	Decomposes to hydrogen chloride gas
N2	N/A	N/A	N/A
Methanol	Strong oxidizers, strong acids and bases, acid anhydrides, acid chlorides	Water, Ethanol, Ether, Acetone, Chloroform	N/A
MEK	Alkali hydroxide, chromium (IV) oxide, oxidizers, nitric acid, sulphuric acid, hydrogen peroxide	Different plastics	Peroxides
Copper Acetate	Strong oxidizers	N/A	N/A
4-NPN	Strong oxidizing agents, strong bases	N/A	Produces nitrous oxides, carbon dioxides
3-PDP	Acid chlorides, acid anhydrides, oxidizing agents	N/A	Carbon oxides
K2CO3	Acids, limes, prolonged contact with aluminum, brass, bronze, copper, lead, tin, zinc or alkali sensitive metals or alloys	N/A	N/A

Appendix AA - Visitor Log Book

Table A30: Example of the Visitor Log book for the site

Name	Position and Company	Reason for Visit	Contact Info	Time In	Time Out	Signature

Appendix AB - Direct and Indirect Labor Calculations

The table shows the calculation of the total number of plant employees (i.e. operators per shift, management, etc.), as well as their calculated salaries.

The number of operators required per shift is given using the formula:

$$NOL = (6.29 + 31.7^2 + 0.23Nnp\ )^{0.5}$$

Where Nnp represents the number of operators required as per the types of equipment within the place and the number of said equipment in the plant. The results are shown below in tables A31 and A32.

Following this, the total operating labour for the plant is calculated by multiplying the calculated N_{OL} by 4.5.

Table A31: Determine Number of Shifting Operators

Equipment Type	Number of Equipment	Number of Operators Required (Nnp)
Batch Reactor	1	1
Nutsche Filter	2	2
Storage Vessel	2	-
Furnace	1	-
Computer Control	1	1
	Total	4
	NOL	3
	Total Operating Labour	14

Table A32: Calculation of Direct Labor Cost and Indirect Labor Cost

Type of Labor	Position	Number of People	Salary per year per person	Total salaries per year
Direct	Operator	14	$55,000.00	$770,000.00
Indirect	QA/QC	1	$52,445.00	$52,445.00
Indirect	Supervisor	3	$61,377.00	$184,131.00
Indirect	Manager	3	$75,061.00	$225,183.00
Indirect	Administrator	1	$41,749.00	$41,749.00
Indirect	Safety and health officer	1	$67,754.00	$67,754.00

Appendix AC - Raw Material Cost

The raw material costs are calculated based on the selected patent examples and industrial scale chemical costs, including freight and insurance. In addition, the yielded percentage, which indicates the total price of the chemical per kg of product, is calculated below. Therefore, a reduction in the cost of 4-NPN can reduce final product cost significantly.

Table A33: Raw Material Cost

Step 1: Production of 4-(3-pentadecyl)phenoxyphthalonitrile Intermediate				
Chemicals	**Quantity**	**Price per kg**	**Total price**	**Yielded Percentage**
3-PDP	502.5g	$16.00/kg	$8.04	10.44%
DMSO	2000mL	$4.50/kg	$8.18	10.62%
Anhydrous potassium carbonate	200g	$1.67/kg	$0.33	0.43%
4-nitrophthalonitrile	250g	$209.00/kg	$52.25	67.85%
HCl	6L	$0.53/kg	$2.65	3.44%
Methanol	4L	$1.10/kg	$5.56	7.21%
Intermediate Costs	558.4g	$137.91/kg	$77.01	100%
Step 2: Production of alkylphenoxy copper phthalocyanine				
Chemicals	**Quantity**	**Price per kg**	**Total price**	**Yielded Percentage**
Intermediate	60.8g	$137.91/kg	$8.39	72.96%
NMP	315mL	$2.95/kg	$0.90	7.85%
Copper acetate	6.24g	$4.30/kg	$0.03	0.23%
DMAE	6.24g	$8.00/kg	$0.05	0.43%
MEK	360mL	$3.68/kg	$1.64	14.30%
N2	500mL	$0.97/L	$0.49	4.22%
alkylphenoxy-CuPc	44g	**$261.20/kg**	$11.49	100%

Appendix AD - Equipment Cost

The table shows the breaking-down cost according to equipment used in the process.

Table A34: Equipment List and Cost

Equipment	Quantity	Average price per unit	Total Price
Storage Tanks	2	$47,500.00	$95,000.00
Batch Reactor	1	$402,416.71	$402,416.71
Nutsche Filter	2	$950,000.00	$1,900,000.00
Batch Weighing system	2	$57,052.73	$114,105.46
Condenser	3	$16,690.35	$50,071.05
Furnace	1	$294,205.56	$54,498.64
Heat Exchanger	1	$40,281.60	$40,281.60
Raw Material Tank	9	$30,663.54	$275,971.86
Hopper	2	$301,908.97	$6,661.34
Bridge crane hoist	1	$2,375.00	$2,375.00
Onsite transport truck	1	$207,900.00	$207,900.00
Fully powered stacker/forklift	2	$8,200.00	$16,400.00
IBC Tote 1	6	$657.00	$3,942.00
Pumps	16	N/A	$158,481.18
Pipeline+Valves (20% of equipment cost)	N/A	N/A	$665,620.97
Total Equipment Cost			**$3,993,725.81**

Appendix AE - Land and Building Cost

The tables below summarize the cost of purchasing land and the building cost for the site.

To estimate the cost of land, a similar piece of land was sourced in Sarnia, ON. To scale this piece of land to the correct size require, the following formula was used:

$$Land\ Price = (Price\ of\ Similar\ Land) \times \left(\frac{Area\ of\ Plant\ Site}{Area\ of\ Similar\ Land}\right)^{0.6}$$

Table A35: Land Purchasing Cost

Area of Plant Site (Acre)	1.71
Area of Similar Land (Acre)	7
Price of Similar Land ($)	$900,000.00
Land Purchasing Price	**$386,350.39**

Table A36: Building Cost

Construction Area	Area m^2	Price per m^2	Cost
XP area	100	$3,000.00	$300,000.00
Non-XP area	1745.62	$2,500.00	$4,364,050.00
Tank Farm	107.38	$800.00	$85,904.00
		Total Cost	**$4,749,954.00**

Appendix AF - Total Fixed Capital Cost

The fixed capital investment can be estimated using Szabo Heuristics, and the detailed formula is listed below including contractor's fee, engineering supervision cost and contingency fee for the new plant.

$$Fixed\ Capital\ Investment(FCI) = Total\ Direct\ Cost(TDC) + Total\ Indirect\ Cost(TIC)$$
$$TDC = 2.2 * Equipment\ Cost + Building\ Cost + Land\ Purchasing\ Cost$$
$$FCI = 2.86 * Equipment\ Cost + 1.3 * Building\ Cost + 1.3 * Land\ Purchasing\ Cost$$

For the total fixed capital investment, we must consider the FCI, working capital, which is required to initiate the chemical plant production process, and consulting fees.

$$Total\ Fixed\ Capital\ Investment = FCI + Working\ Capital + Consulting\ Fee$$

Table A37: Total Fixed Capital Cost Estimation

Expenses	Costs
Fixed Capital Investment (FCI) *Based on Szabo heuristics	$20, 463, 783.96
Working Capital *Two months of raw materials required	9500 kg * $261.24 RMC/kg = $2,481,760.2
Consulting Fee *Refer to appendix B	$23,000
Total Fixed Capital Investment	$22, 964, 454.20

Appendix AG - Manufacturing Cost

The table shows the annual manufacturing cost breakdown, estimating factors and cost percentage accordingly. From the chart below, it indicates that the RMC dominates the annual manufacturing cost; as a result, if the RMC can be reduced by negotiating chemicals' price, the annual manufacturing cost can be reduced as well.

$$Annual\ Cost = Cost\ of\ Basis * Predetermined\ Factor$$

Table A38: Manufacturing Cost Break-down

Content	Basis	Factor	Annual Cost	Yielded Percentage
RMC	RMC	1	$13,061,895.97	66.07%
Operating Labor	Operating Labor	1	$770,000.00	3.89%
Maintenance	Fixed Capital Investment	0.06	$1,377,867,.25	6.97%
Local taxes	Fixed Capital Investment	0.02	$459,289.08	2.32%
Insurance	Fixed Capital Investment	0.01	$229,644.54	1.16%
Direct Supplies (PPE, computer, office)	Operating Labor	0.3	$231,000.00	1.17%
Overhead plant cost	Supervisor and manager salaries	1	$571,262.00	2.89%
Sales cost	Sales revenue	0.04	$1,400,000.00	7.08%
Bonus	Salaries	0.2	$268,252.40	1.36%
Utilities	Process Equipment	1	$384,840.00	1.95%
Waste disposal	Waste disposal	1	$988,991.55	5.00%
Nitrogen	Nitrogen	1	$28,098.00	0.14%
Total annual manufacturing cost			**$19,771,140.79**	**100%**

Appendix AH - Cash Flow

The table summarizes the total fixed capital investment, depreciation value, net income and annual manufacturing cost. The depreciation factor is 30%, and with half-year rule, the first year's price is depreciated by 15%, and by 30% for the rest 4 years. The taxation is typically 45%, and profit is calculated as income after tax. As setting up 10% MARR value, future price is brought to the present value to calculate the cumulative cash flow, which is helpful to determine the payback period. At the end of the chemical plant, the salvage value is estimated as $700,000 since the land price will not be depreciated as time passes.

Table A39: Annual Cash Flow and Net Present Value

Year	Fixed Capital Investment (MM$)	Depreciation Value (MM$)	Remaining Value (MM$)	Revenue (MM$)	Annual Costs (MM$)	Profit (MM$)	Cash Flow (MM$)	Discounted Cash Flow (MM$)	Discounted Cumulative Cash Flow (MM$)
0	$13.78	/	/	/	/	/	-$13.78	-$13.78	-$13.78
1	$9.19	/	$22.96	/	/	/	-$9.19	-$8.35	-$22.13
2	/	$3.44	$19.52	$35.00	$19.77	$9.93	$9.93	$8.20	-$13.93
3	/	$5.86	$13.66	$35.00	$19.77	$11.01	$11.01	$8.27	-$5.65
4	/	$4.10	$9.56	$35.00	$19.77	$10.22	$10.22	$7.68	$2.03
5	/	$2.87	$6.70	$35.00	$19.77	$9.67	$9.67	$6.60	$8.63
6	/	$2.87	$3.83	$35.00	$19.77	$9.67	$9.67	$6.00	$14.63
7	/	$3.83	/	$35.00	$19.77	$10.10	$10.10	$5.70	$20.33
8	/	/	/	$35.00	$19.77	$8.38	$8.38	$4.30	$24.63
9	/	/	/	$35.00	$19.77	$8.38	$8.38	$3.91	$28.54
10	/	/	/	$35.00	$19.77	$8.38	$8.38	$3.55	$32.09
11	/	/	/	$35.00	$19.77	$8.38	$8.38	$3.23	$35.32
12	/	/	/	$35.00	$19.77	$8.38	$8.38	$2.94	$38.25
13	/	/	/	$35.00	$19.77	$8.38	$8.38	$2.67	$40.92
14	/	/	/	$35.00	$19.77	$8.38	$8.38	$2.43	$43.35
15	/	/	/	$35.00	$19.77	$8.38	$8.38	$2.21	$45.55
16	/	/	/	$35.00	$19.77	$8.38	$8.38	$2.01	$47.56
17	/	/	/	$35.00	$19.77	$8.38	$8.38	$1.82	$49.38
18	/	/	/	$35.00	$19.77	$8.38	$8.38	$1.66	$51.04
19	/	/	/	$35.70	$19.77	$8.76	$8.76	$1.58	$52.61

Appendix AI - Received Quotes

*Attached all received quotes

Appendix AJ - Safety Data Sheet (SDS)

*Attached all SDS used in the design of this process