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Dear Professor Bruce Vrana and Dr. Warren Seider,

The following report contains a proposed process design for the production of polyhydroxyalkanoates (PHAs) from the microalgae strain *Scenedesmus* sp. PHA, a biodegradable polymer, which would serve as a viable sustainable alternative to traditional petroleum-based polymers if it can be produced in an economically viable manner.

Our process has the capacity to produce 8,367 US tons per year of PHAs, as well as byproducts — 29,283 US tons of de-oiled biomass, and 4,183 US tons of lipid (triolein). This process utilizes flue gas from a natural gas power plant as the carbon source and anaerobic digestion centrate (ADC) from a wastewater treatment plant as the nutrient source.

The primary goal of this report was to achieve a 15% internal rate of return (IRR), so rigorous profitability analysis was performed. However, with a total capital investment of $392.1 million and an annual profit margin of $19.3 million, it is concluded that the project is not reasonably economical. The internal rate of return was 1.6% with reasonable selling prices of the products. For this reason, we don't recommend moving forward with this design unless significant changes are made, including reductions in operating costs and/or increases in byproduct selling prices.

Sincerely,

Emma Schultz   Akaash Padmanabha   Luis Martinez-Banegas

Production of PHAs from Microalgae

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Abstract

Biodegradable polymers are becoming an attractive alternative to traditional petroleum-based polymers; namely, polyhydroxyalkanoates (PHAs) are naturally occurring biodegradable polyesters synthesized by various microorganisms and are one of the most promising sustainable plastic alternatives in the market. PHAs can be produced naturally by bacteria or algae without diverting crops and can biodegrade in landfills or even marine environments. This project produces PHAs from the microalgal species *Scenedesmus*, employing the use of flat plate photobioreactors for algae cultivation, gravity settling and centrifugation for harvesting and dewatering, microbubble extraction for cell lysis, and a separation train for the purification of PHA from lipids. The annual production capacity is 8,367 US tons of PHAs, 29,283 US tons of de-oiled biomass, and 4,183 US tons of lipid (triolein), with the primary goal of achieving a 15% internal rate of return (IRR). However, with a total capital investment of $392.1 million and an annual profit margin of $19.3 million, this project fails to meet the desired economical outcome. The internal rate of return was 1.6% when using reasonable selling prices for the products but showed promise with a reduction of capital costs (e.g., reduction in algal photobioreactor costs) or an increase in the profit margins (e.g., increase in PHA selling price or reduction in utility usage).

Introduction

Background

Polymers currently account for 6% of global fossil fuel consumption (Ellen MacArthur Foundation, 2016). This number is projected to increase to 20% by 2050. The U.S. is the primary global generator of plastic waste (Law, et al., 2020). In Figure 1, plastic end destinations show that recycling is not as common of an end destination as people may believe, with only 9% of plastics being recycled (U.S. EPA, 2020). 75% of plastic ends up in landfills, where they take anywhere from 20 years to over 500 years to break down (World Wildlife Fund, 2021).

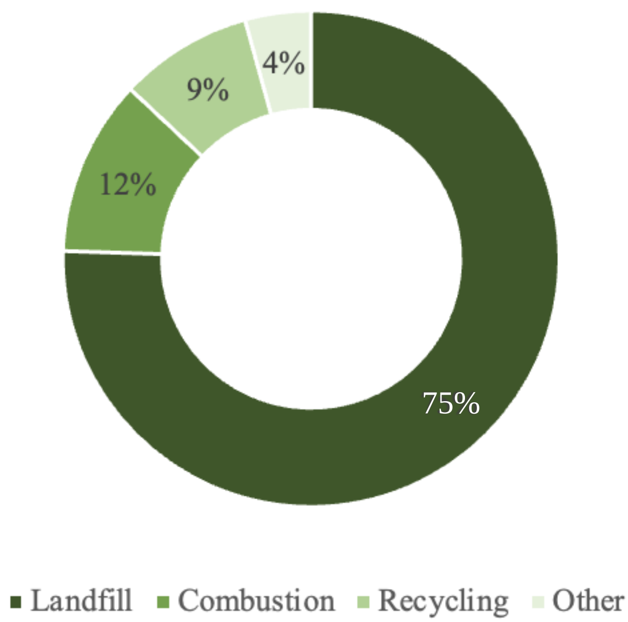


Figure 1. Plastic End Destinations *(U.S. EPA, 2020)*

Considering the harsh reality of this situation, it is becoming increasingly necessary to look for viable alternatives to traditional petroleum-based polymers. Many bioplastics that are currently in the market, such as polylactic acid (PLA), are not truly sustainable alternatives, as they are biodegradable only in industrial facilities and often divert crops. Other bioplastics have similar disadvantages, and some are even made from petroleum (Verbruggen, 2021). Polyhydroxyalkanoates (PHAs) are an appealing alternative to these bioplastics. PHAs are naturally occurring biodegradable polyesters that are synthesized by various microorganisms. These are the most promising sustainable plastic alternative in the market — they can be produced naturally by algae without diverting crops and can biodegrade in landfills or even marine environments (Costa, 2019).

This report aims to synthesize PHA naturally from green microalgal biomass in nutrient-depleted environments. Microalgae are photosynthetic microorganisms, which are classified into two categories of prokaryotes and eukaryotes. Prokaryotic microalgae such as cyanobacteria are known as blue-green algae, and eukaryotic microalgae comprise diatom and green algae. Green algae, which will be used here, are unicellular eukaryotes with cell walls.

Green algae grow through mixotrophic metabolism (Smith et. al., 2015). This is a two-stage growth regime, which includes growth and starvation phases. The growth phase is heterotrophic growth — it requires an organic compound which will serve as both the energy and carbon source. The most frequently used organic carbon compound is glucose, but other carbon sources can also be used. This phase occurs when organic carbon content is high. Heterotrophic, colorless taxa are present to carry out this phase. The starvation phase is photoautotrophic growth — it requires CO_2 (carbon source) and light (energy source). This occurs with nutrient deprivation and begins with the induction of photosynthesis, usually when the carbon content is low. Chlorophylls, present in chloroplast, are the main photosynthetic pigments (Smith et. al., 2015).

Recently, researchers (Garcia et al., 2021) have reported that PHA is produced from the unique green microalgal species *Scenedesmus*. They studied critical nutritional parameters that result in increased PHA accumulation within algae cells — PHA accumulation occurs naturally in photosynthetic organisms, but their yield can be increased under nutrient-deficient conditions in the presence of a carbon source. *Scenedesmus* doesn't require supplementation with large amounts of exogenous carbon to produce PHA, which is an economical advantage over use of higher accumulating bacteria. It has high tolerance to salinity stress, which makes cultivating it in seawater or wastewater possible. It also produces other valuable metabolites such as lipids and carbohydrates, which are macromolecules of interest to produce biofuel and bioethanol.

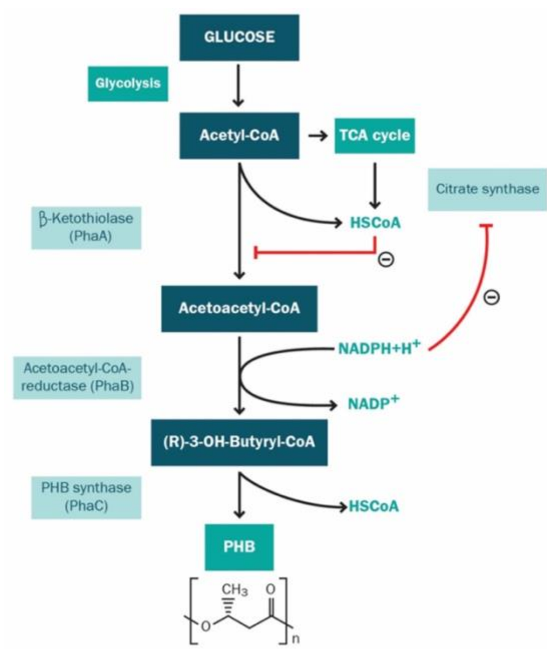


Figure 2. Synthesis pathway of PHA *(Garcia, et al., 2021)*

As shown in Figure 2, the synthesis of PHA in photosynthetic organisms begins with the consumption of acetyl-CoA, which is formed in a glycolysis fermentation of glucose. Two acetyl-CoA molecules then form an acetoacetyl-CoA molecule in a condensation reaction catalyzed by beta-ketothiolase (PhaA). This molecule is reduced to R-3-hydroxybutyryl-CoA by nicotinamide adenine dinucleotide phosphate (NADPH-dependent acetoacetyl-CoA reductase (PhaB). Lastly, PHB synthase (PhaC) catalyzes the binding of R-3-hydroxybutyryl to an existing polyhydroxybutyrate (PHB) molecule through an ester bond, releasing HSCoA. The chemical composition of the PHA polymers which result can be varied by changing the subtrates fed to the *Scenedesmus* sp. algae. Since the synthesis of PHA is regulated at the enzymatic level, the intracellular concentration of acetyl-CoA and free CoA is central in the synthesis of PHA. The enzymatic activity and availability of the precursors to PHA are dependent of the presence of different carbon compounds (e.g. glucose, glycerol) in the growth medium (Garcia, et al., 2021). In our process, this pathway occurs during the growth phase, when glucose is present after being produced during photosynthesis.

The following process considered the laboratory data of Garcia et al. (2021) to scale-up an industrial process that utilizes photobioreactors, and light and nutrients for the cultivation of algae biomass and accumulation of PHA within the cells. It will also employ techniques for biomass harvesting and dewatering, cell disruption for recovery of metabolites, and separation to recover PHAs. Furthermore, characterization techniques will ensure that the resulting copolymers have the desired polymer properties, which include average molecular weight, glass transition and melting range (Bejagam, 2021).

Motivations and Goals

The principal motivation for this project is the global plastic crisis, as discussed above. Our goal is to produce PHA, an alternative that minimizes both upstream and downstream impacts. The main barrier which could prevent the widespread use of PHA is that production costs of petroleum-based polymers are lower than biodegradable alternatives. Therefore, we aimed to execute this project with a 15% internal rate of return (IRR) (Costa, 2019). This can be achieved by using co-products to offset production costs, which also furthers the sustainability of our process by limiting waste products. Our project also aimed to be as sustainable as possible by recycling raw materials and using waste streams from other process plants as alternatives for raw material inputs when available.

Objective-Time Chart

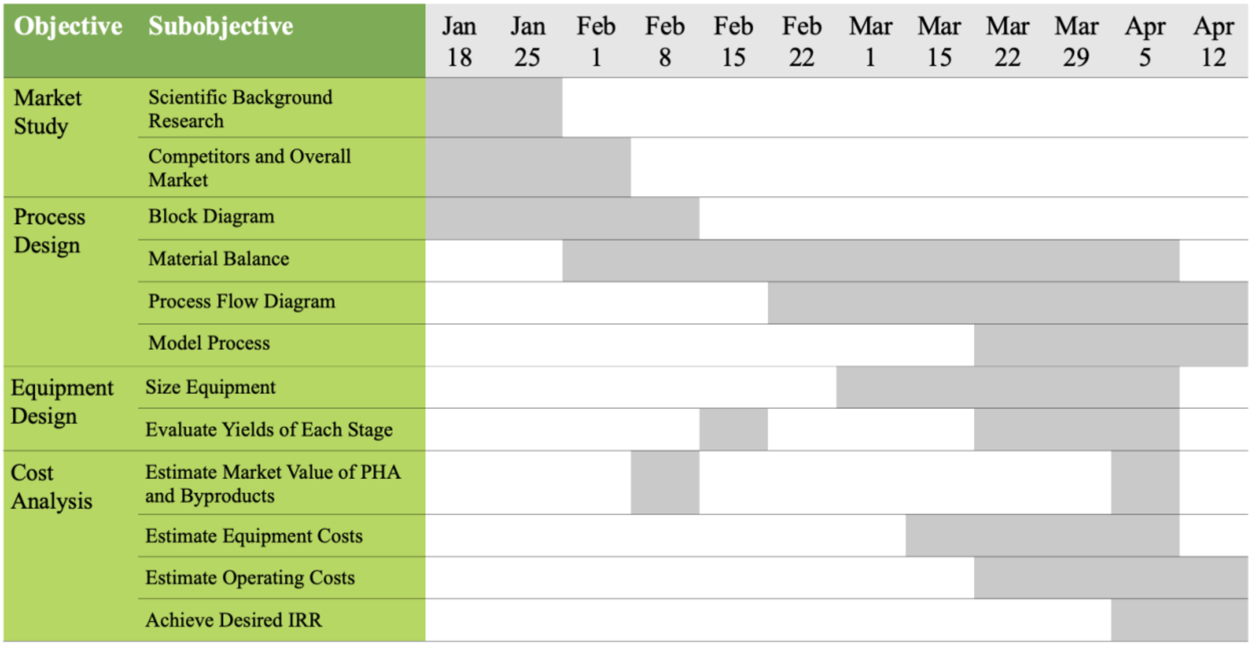


Figure 3. Objective-Time Chart

Market and Competitive Analysis

The global market size for plastics is $580 billion (Grand View Research, 2021) and the market size for biodegradable plastics is $2.8 billion (Tiseo, 2021). Bioplastics also make up about 10% of the market share (Ponnappan, 2021; Maurya, 2016), but those are not necessarily biodegradable. Non-biodegradable bioplastics may be diverting crops without a sufficient sustainable outcome to justify it, while biodegradable bioplastics made from petroleum feedstocks are unsustainable as well. Our product would enter the PHA market, which is a polymer that is both bio-based and biodegradable.

Currently, two main players in the biodegradable plastics market are Danimer Scientific and Mango Materials. Danimer Scientific has a market cap of $578 million (CNBC, 2022), which gives it an approximate market share of 20%. Danimer Scientific recently acquired Novomer, a leading producer of carbon-neutral materials and feedstocks to produce biodegradable materials, including PHA-based resins (Bioplastics Magazine, 2021). It currently operates out of a plant in Winchester, Kentucky, with an annual production rate of 10,000 tons per year (Tullo, 2020). It utilizes a fermentation process in which canola oil is consumed by soil bacteria to produce PH3P, a type of PHA. This is then processed into a powder form to be sold. Danimer has a patent for the PHA that comes from this process — Nodax PHA. Nodax PHA has been shown to biodegrade at a similar rate to cellulose powder or wood pulp in a proper waste management setting. It can also be effectively processed with organic waste in a landfill. Nodax PHA should begin to biodegrade over the course of six months in ocean water. It is also FDA approved for food contact (Bioplastics Magazine, 2018).

Mango Materials, another competitor, co-locates with methane producers to convert methane to PHA using bacteria (Mango Materials, 2022). This process grows bacteria in fermenters, with inputs of methane, oxygen, and nutrients. The PHA-rich bacteria are removed from the fermenter, after which the polymer is separated from the rest of the cell mass. These plastics can be anaerobically degraded to produce methane gas, which closes the loop by providing feedstock for this PHA production process. By using methane instead of sugar as a carbon feedstock, Mango Materials sees a lot of cost savings. This plant has a production rate of 1,000 US tons per year of PHA (Morse, 2014).

There are existing customers in the market for PHA, including P&G, Biomers, Metabolix, and Bacardi, which represent various industries, such as packaging, nanotechnology, and medical and pharmaceuticals (Chen, 2009). Use cases for PHA include shampoo bottles and food and beverage packaging for the packaging industry, compostable batteries for the nanotechnology industry, and sutures for the medical and pharmaceutical industry (Chen, 2009).

Our main differentiation from competitors is our usage of algae instead of bacteria. As mentioned in the "Background" section, *Scenedesmus* offers unique value even in comparison to other algae strains. Its relatively low need for exogenous carbon in order to produce PHA makes the production costs lower, making it ideally possible to offer lower pricing as compared to other algae strains. The theoretical advantage of this method compared to bacteria is that it doesn't divert resources such as canola oil in order to produce PHAs. The saturation of customers in the market for biodegradable plastics, the relatively small current market size, and the potential value addition and differentiation of *Scenedesmus* makes this a compelling market entry case.

However, the significant land usage for algae cultivation, along with the cost of photobioreactors (PBR) is a large disadvantage compared to PHA production with bacteria. Despite this, a process was still designed with *Scenedesmus* algae in alignment with the project problem statement (see Appendix).

Customer Requirements

PHAs have many unique properties that make them a desirable product to customers in various industries. Certain PHAs are biocompatible, which makes them useful in medical and pharmaceutical applications, such as sutures, cardiovascular patches, drug delivery carries, and implants (Garcia, et al., 2021). PHAs are also blend-able and have good mechanical properties, so they can be applied in nanotechnology, in products including films, compostable batteries, nanoparticles, and nanocomposites (Garcia, et al., 2021). Their strong barrier properties are necessary for single-use packaging food, beverages, and consumer products (Kolvalcik, 2019). Most importantly, PHAs are biodegradable. Generally, they can decompose in 18 months if in an environment with microbial activity (Danimer Scientific, 2021).

Our product will target the packaging industry, as other industries require the consideration of other properties such as biocompatibility and mechanical properties. Therefore, our primary consideration is biodegradability, which is an inherent property of PHA. The PHA is sold as pellets, which allows it to serve as a base input for the production of packaging.

It is also important to consider customer requirements for our byproducts: de-oiled microalgal biomass (DMB) and lipids. DMB is rich in carbohydrates, proteins, and minerals. It can be used as a feed, fertilizer, and substrate for the production of bioethanol and biomethane. Thermochemical conversion of DMB also results in fuels and industrial chemicals. Future applications of DMB may include conversion into novel biomaterials such as nanoparticles. The lowest value application of DMB is use in adsorption of dyes and heavy metals from industrial effluents (Maurya, 2016).

The carbon to nitrogen ratio determines the most beneficial use case of the DMB. High C/N ratios make DMB useful for biofuel production, while low C/N ratios, representative of high protein content, make DMB useful as a fertilizer or fermentation medium (Maurya, 2016).

Flocculation by chemical methods and extraction with organic solvents may make DMB unfit for various use cases. However, flocculation with chemical methods was not the chosen dewatering technique in our process, and organic solvents are only used downstream in the process after DMB extraction (Maurya, 2016).

The other byproduct of our process is a lipid, which has been assumed to be triolein since it is the most common triglyceride in algae biomass (Zapata-Boada et. al., 2022). Triolein can be used for personal care products. It can also be used as a lubricant in the textile, cosmetics, or drugs industries, and as an emulsifier for water/oil mixtures (National Library of Medicine, 2022). Triolein also has various applications in the food and beverage industries, including its use as an emulsifying agent for the production of candy (Chemical Book, 2022). Also, triolein can be trans esterified with methanol to make biodiesel and omega-3 fatty acids (Stokes, 2020).

Due to the contact of the triolein with chloroform in our process, it will most likely not be safe for industries which create products that will be ingested or make contact with skin. However, it can still be sold to the textile industry for use as a textile finishing agent or an additive in pigment grind (Chemical Book, 2022).

Preliminary Process Synthesis

The main goal of this project is to produce PHA using *Scenedesmus* sp. algae (Garcia, et al., 2021) in an economically viable manner by scaling up cultivation, dewatering, extraction, and purification steps to industrial scale. Byproducts — lipids and de-oiled microalgal biomass (DMB) — will also be isolated in the process. In order to design the different portions of this process, many decisions were made, with alternatives considered, as detailed in this section.

Algal Cultivation

Important decisions for the first portion of our process include water source, nutrient source, and photobioreactor type.

Water Selection

Freshwater, wastewater, and seawater were considered as options for the water source in the algae cultivation process. Despite the tolerance of *Scenedesmus* to salinity stress, seawater was eliminated because of the detrimental effect that salt would have on the equipment.

There are many potential benefits attributable to the use of wastewater in algae cultivation. Wastewater contains nutrients necessary for algae growth. The ammonia and phosphate concentrations in wastewater typically range from 400 to 800 mg/L and 20 to 60 mg/L, which would be desirable for the process due to the required nutrient inputs (del Mar Morales-Amaral, 2015).

Despite the benefits of wastewater, it was also eliminated as a potential water source due to the variability in content and possibility of contamination. Process water (freshwater) was selected for the process. The water demands for cultivation are high, so in order to minimize water waste, the majority of water used throughout the process will be recycled.

Nutrients and Carbon Source

In addition to the carbon source that is a direct input to the algal process of PHA production, micronutrients/elements such as nitrogen, phosphorus, and iron also affect the productivity in a non-trivial manner. Based on a lab study performed on PHA growth with *Scenedesmus* sp. algae, we performed a cost analysis on PHA yields compared to various nutrient inputs (Garcia, et al., 2021). Due to the high cost of nitrogen, an alternative source to pure inputs was desirable.

Table 1. Nutrient Cost Analysis

Run	Glucose (g L−1)	Nitrogen (mM)	Phosphorus (mM)	Iron (mM)	Salinity (g L−1)	PHA (% w/w)	PHA (g L−1)	Cost ($/L)	g of PHA/$
1	1	0	0	0	0.5	9.793	0.064	37.07	0.0017
2	1	0	0	0.021	2	26.25	0.171	37.39	0.0046
3	1	0	0.23	0	0.5	11.68	0.082	37.88	0.0022
4	1	0	0.23	0.021	2	9.075	0.073	38.21	0.0019
5	1	17.6	0	0	2	13.8	0.104	77.05	0.0013
6	1	17.6	0	0.021	0.5	29.92	0.239	77.15	0.0031
7	1	17.6	0.23	0	2	12.2	0.085	77.86	0.0011
8	1	17.6	0.23	0.021	0.5	8.612	0.06	77.97	0.0008
9	4	0	0	0	2	13.08	0.052	37.48	0.0014
10	4	0	0	0.021	0.5	17.14	0.12	37.58	0.0032
11	4	0	0.23	0	2	11.6	0.087	38.29	0.0023
12	4	0	0.23	0.021	0.5	8.135	0.049	38.40	0.0013
13	4	17.6	0	0	0.5	0.831	0.007	77.24	0.0001
14	4	17.6	0	0.021	2	10.75	0.134	77.56	0.0017
15	4	17.6	0.23	0	0.5	2.267	0.014	78.05	0.0002
16	4	17.6	0.23	0.021	2	2.959	0.03	78.38	0.0004

As shown in Table 1, the trials which included nitrogen input were exceedingly expensive, with high costs per liter and low PHA production rates per dollar spent. This led us to consider alternatives to purchasing each nutrient input as a raw material. Despite rejecting wastewater as a water source for cultivation, it was determined that the preferable nutrient source would be Anaerobic Digestion Centrate (ADC), which is an economical fertilizer substitute produced in the wastewater treatment process. It provides all the nutrients that are necessary for microalgal growth (Bohutskyi, 2016).

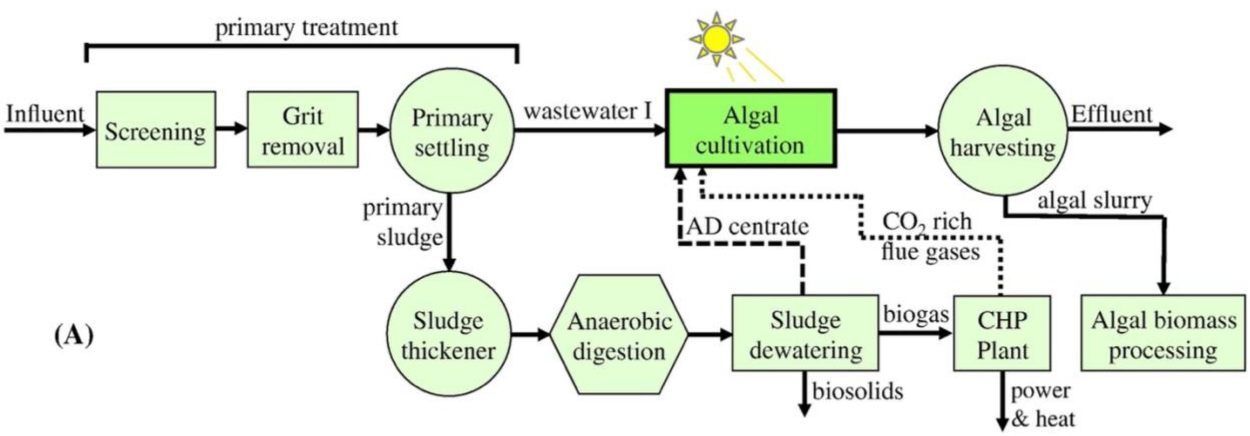


Figure 4. Block Flow Diagram for Primary Wastewater Treatment *(Bohutskyi, 2016)*

Figure 4 shows a block flow diagram for primary wastewater treatment, which produces anaerobic digestion centrate. This can be fed to the algae cultivation block of our process as a nutrient input (Bohutskyi, 2016).

30% ADC was found to be optimal for the growth of *Scenedesmus* sp. (del Mar Morales-Amaral, 2015). On average, ADC contains nitrogen, phosphorus, and potassium concentrations of 1,000 mg/L, 225 mg/L, and 200 mg/L, respectively (Herrera, 2009). Furthermore, the ratios necessary for biomass production are 2:1 carbon dioxide, 1:20 nitrogen, 1:100 phosphorus, by weight (Acien F. , 2012) (del Mar Morales-Amaral, 2015). The ADC contains the necessary amount of nutrients, so supplementation of nutrients in addition to the ADC is not necessary. One concern with the use of ADC was the presence of wastewater bacteria, but this proved to be insignificantly antagonistic to the growth of the *Scenedesmus* algae. Although a large amount of ADC is now being supplied to the culture, there still exists a lack of carbon source for proper algal growth. Pure carbon dioxide and glucose are both incredibly expensive consumables, so it is common for pilot and commercial scale plants to co-locate with industrial process plants and use their flue gas to reduce the cost of CO_2 to as low as zero (Acien F. , 2012). We intend to do the same for our process.

Photobioreactor Selection

When selecting a photobioreactor (PBR) for use in algae cultivation, the first consideration was comparing open and closed systems. Many options for each exist in practice today. Closed systems are associated with reduced risk of contamination, low CO_2 loss, smaller area requirements, and higher productivity rates. However, they are also some downfalls: They are harder to clean than open systems; the tube material can partially decrease sunlight penetration; the system must be cooled and degassed effectively because any excess O_2 production can reduce growth; the cost of construction is about one order of magnitude higher. Closed systems include horizontal tubular, vertical tubular, and flat plate (also known as flat panel) photobioreactors. Open systems include open raceways and thin layer.

Thin layer raceways are shown to have higher productivity than open raceways, so that was deemed to be an optimal open system (del Mar Morales-Amaral, 2015). However, despite the several negative implications of closed systems, they were selected due to lowered risk of contamination and significantly higher productivity per area of land.

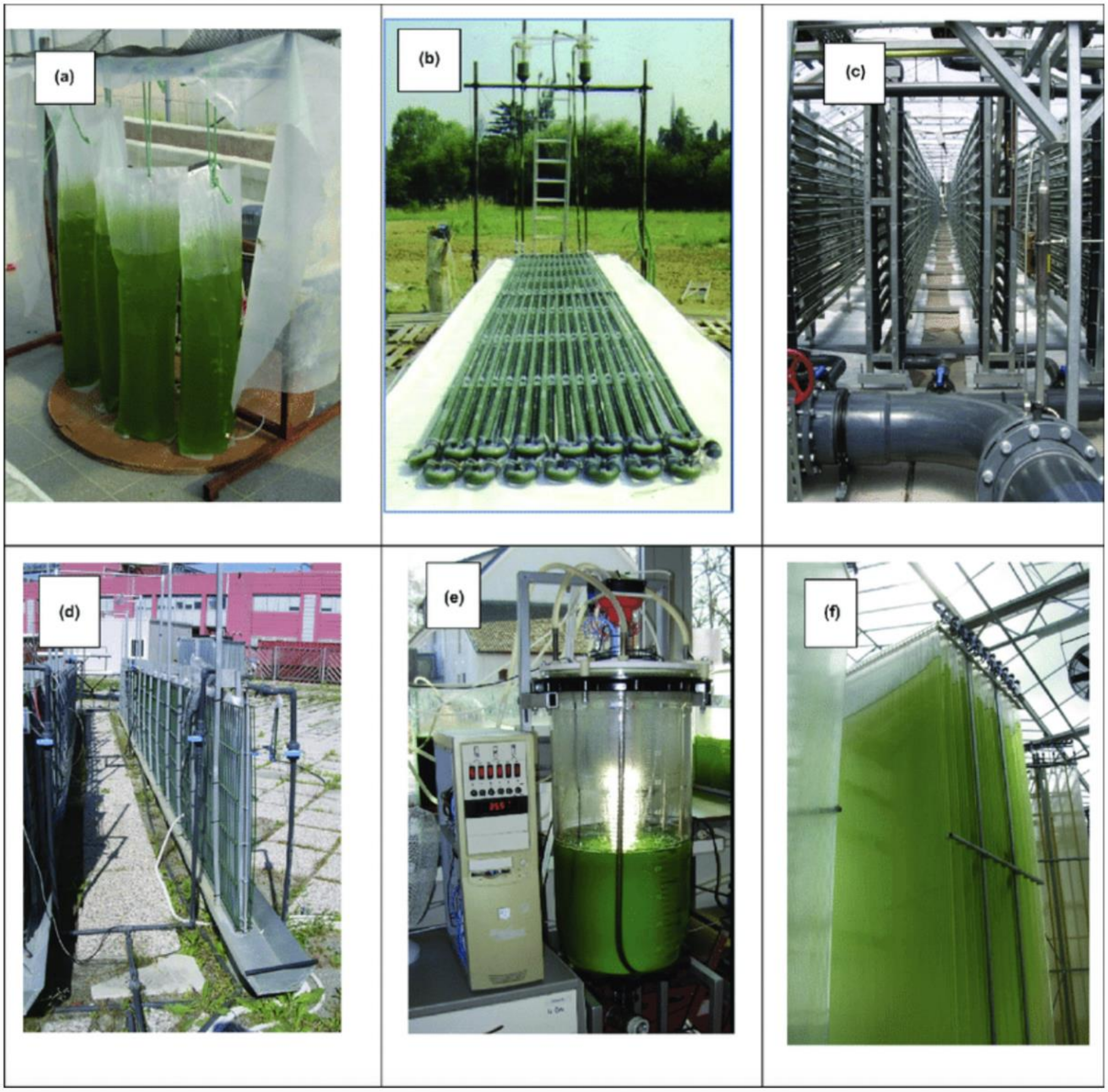


Figure 5. Types of Closed Photobioreactor Systems *(Masojidek & Torzillo, 2008)*

Shown in Figure 5, closed PBR types include (a) hanging plastics bags, (b) horizontal tubular, (c) vertically stacked tubular, (d) vertical flat-plate, (e) annular column, and (f) hanging flat-plate (Masojidek & Torzillo, 2008).

Annular column PBR systems are not practical on industrial scale. Vertical PBRs showed higher areal productivities and photosynthetic efficiencies compared to horizontal systems (de

Vree, 2015). Hanging plastic bag systems, although a vertical system, have a very high operating cost: 31.4% in one study (Zhu, 2018). Tubular photobioreactors are better for lighting, while flat plate photobioreactors are better for cost per volume, liquid mixing, oxygen accumulation, and maintenance (Cuello, 2016).

For these reasons, flat plate photobioreactors were selected for this project. Flat plate PBRs are considered one of the most robust PBR designs. They have been employed for decades, so the process is well-documented (Posten, 2009) (Clippinger & Davis, 2019). Areal productivity is highest in flat panel PBRs (Slegers, 2013). They also have a relatively high photosynthetic efficiency of 3.8% (de Vree, 2015).

Harvesting

Harvesting is performed at the site of algal cultivation in the bottom circulation tank. This also serves as a preliminary dewatering step. Gravity settling was chosen as the harvesting method. This was selected over several other options, including filtration and chemical flocculation. Filtration is most suitable for small systems and works efficiently if the incoming algae slurry is already at 3-4 wt% biomass, which is not the case in this process. Chemical flocculation, while an effective method, was eliminated due to the difficulty of removing the flocculants, such as aluminum and ferric cations, aluminum sulfate, and ferric chloride. Removing these chemicals from the separated algae makes the process inefficient and expensive for commercial use (Katuwal, 2017).

Spontaneous gravity settling, also known as bioflocculation, is highly strain-specific, and is known to work well for *Scenedesmus*. As designed, it will be able to increase the algae concentration to around 1 wt% of the algae slurry (Davis et. al., 2016). This minimizes the unreasonable operating cost of directly inputting the extremely dilute culture into the centrifuge, reducing the volumetric flow rate into the centrifuge to 20 times less than if gravity settling had not occurred.

Dewatering

After the transportation of harvested algae to the indoor process plant, the main dewatering step occurs. Dewatering is a crucial part of PHA production because for cell lysis to occur, the concentration of algae in the mixture must be much higher than what results in the cultivation step. Utilizing thermal methods alone has been shown to be environmentally unfavorable when compared to mechanical dewatering methods (Mediboyina, Banuvalli, & Chauhan, 2020).

Because of the requirements of the following extraction stage, it is necessary to concentrate the dilute algae solution to 94% weight by water (w/w) to proceed to the extraction stage (Yadav, et al., 2021). Initially, a self-cleaning disc stack centrifuge was selected for the high throughput needs of the process (Grima, 2003). A small amount of water bypass would further decrease the load of the system (both capital and operating cost), with an operational mode that is continuous suspension and discontinuous concentrate. This method reduces the water concentration in the algae slurry to 88%, with an energy consumption of 1 kWh of energy is consumed per 1 m^3 of liquid (Grima, 2003). Because of the requirements of the following extraction stage, it is necessary to concentrate the dilute algae solution to 94% weight by water (w/w) to proceed to the extraction stage (Yadav, et al., 2021).

Later in the decision-making process, this centrifuge was replaced with another centrifuge that could withstand a much higher flowrate and minimize the necessary number of centrifuges to 1. This centrifuge is a bowl centrifuge that can increase the algal concentration to 20% (i.e., 80% weight by water) (Davis, et al., 2016). Thus, the combination of a higher capacity as well as a larger liquid bypass flow rate proved to be extremely advantageous.

Extraction

After centrifugation, extraction is the next step in order to lyse the cells and release the products. Following the evaluation of various alternatives, including bead beating with solvents such as chloroform, microbubble extraction was selected as the extraction technique for this process (Yadav, et al., 2021) (Krehbiel, 2014). Cell disruption is usually necessary in order to recover intracellular products from microalgae — ultrasonication of suspended microalgal cells can be used to disrupt biomass (Grima, 2003). Microbubble extraction was chosen because of its lowered energy consumption, as well as its improved separation/recovery of products and its lack of a solvent requirement (Krehbiel, 2014) (Yadav, et al., 2021).

The heat of combustion of algal biomass is $2.7 * 10^7$ J/kg. Current cell disruption techniques usually result in a net negative energy balance. Energy requirements for typical cell disruption techniques range from $3.3 * 10^7$ J/kg of dry biomass for hydrodynamic cavitation to $5.3 * 10^8$ J/kg for high-pressure homogenizers. The selected extraction technique for our process, microbubble extraction, does not result in a net negative energy balance. Microbubble generation requires $6.17 * 10^6$ J/kg of dry biomass (Krehbiel, 2014).

Furthermore, this process was clearly laid out in the research of Yadav, et al. (2021). The water-algae mixture was input at 94 wt%, as listed in the literature, so that the same metrics and calculation procedures could be used (Yadav, et al., 2021).

Purification

The lipid-PHA mixture that comes out of the extraction unit must be separated in order to obtain a pure PHA product. This will be done by feeding in chloroform, methanol, and water, as discussed in various literature and performed in a laboratory experiment by PhD candidate Owen Land. This process was chosen after considering various separation trains and solvents, including cyclohexanone. These solvents were chosen due to the existence of material balance information and solubility with PHA and triolein.

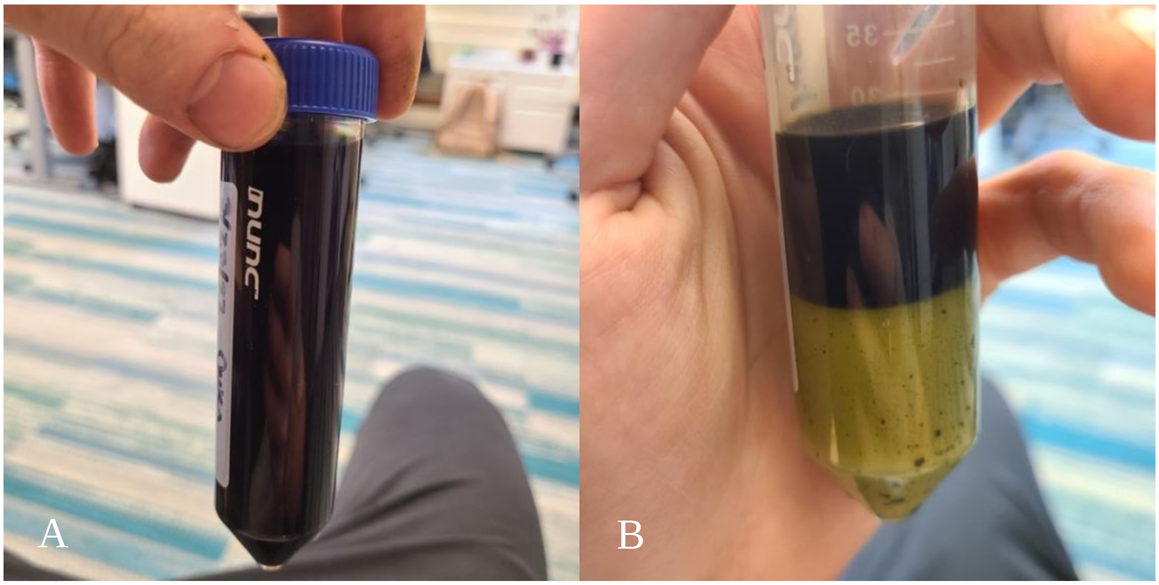


Figure 6. Laboratory Results for Separation Design *(Land, Unpublished, 2022)*

In the experiment, Land added methanol and cyclohexane together, obtaining two separate phases. However, upon the addition of lipid, it dissolved very well into both phases, creating a mixture that was entirely dark green, as shown above in Figure 6a. This is because you can't have two pure solvents with the lipid. After adding water to the mixture, a phase separation was forced — the water goes with the methanol and the lipid goes with the cyclohexane, as displayed in Figure 6b.

Later in our design of the separation train, the cyclohexane solvent was substituted with a chloroform solvent due to further availability of ratios of addition. This follows typical Folch extraction, which is one of the most popular techniques to isolate lipids from biological samples. It uses a biphasic solvent system made up of chloroform, methanol, and water (Eggers & Schwudke, 2016). Volumetric ratios of 9:1 methanol to chloroform and 1:1 methanol to water were used for this process (Salim, 2009) (Land, Unpublished, 2022).

In the designed process, after the addition of water, the liquid phases separate into triolein-chloroform and methanol-water. It was determined that a decanter was necessary after the addition of water in order to create a quiet zone before the separation of the two phases into distillation columns. Due to the large amount of methanol and water, four distillation columns were used in parallel for the separation of methanol and water. Although this split resolved the issue of having an excessively oversized column (initially over 12 meters in diameter), the low energy efficiency remained an issue since the total flow through reboilers and condensers was unchanged. Another distillation column was used for the separation of the chloroform and triolein, which proved much less problematic with regards to the utility cost (with a lower flow rate). However, because of the presence of a lipid with an extremely high boiling point (over 600˚C), the purity of the bottoms stream was limited by the temperature of the high-pressure steam used in the kettle vaporizers (at 250˚C). Because the triolein stream is removed from the entire separation train (independent from the other unit operations), the final purification of the triolein byproduct is outside the scope of this study. On the other hand, the water, methanol, and chloroform are recycled in an effort to reduce operating costs, with fresh inputs of each being reduced by 100X due to each stream being over 99% pure.

Characterization of PHA

The type of PHA produced by any process varies depending on the carbon source (Kniewel, 2017). Generally, there are short chain length (scl) and medium chain length (mcl) PHAs, which have different material properties and subtypes: scl-PHAs include PHB and PHBV and mcl-PHA is known as PHA. PHBV is known to be higher quality and biocompatible, as necessary for pharmaceutical applications (Strong, 2016). Danimer Scientific and Mango Materials are both strong players in the biodegradable polymer market, and both produce mcl-PHAs. Due to the nature of mixotrophic metabolism (with both simple carbon sources and glucose used by the algae), our process will likely produce both scl-PHA and mcl-PHA. Since we are targeting the packaging industry with our product, the production of the lower quality mcl-PHA, specifically PH3B, will not be problematic (Costa, 2019), (Chen, 2009).

The method selected for characterization of PHAs is Fourier Transform Infrared (FTIR) Spectroscopy (Leong, et al., 2017), (Mal et. al., 2022). A sample of the final PHA product will be taken every 8 hours to perform FTIR Spectroscopy for quality control. FTIR analysis is a subset of infrared microscopy. It is used in order to determine different bonds in molecular segments. A monochromatic ray of infrared wavelength is sent through the sample. The transmission is recorded in a crystal detector, which performs a Fourier transform to produce a spectral fingerprint. From this, the molecular architecture of the sample can be predicted (Mal, et al., 2022).

Plant

Location

Since the cultivation of algae is conducted outdoors, ambient conditions are significant to the productivity of the overall process. In terms of temperature, *Scenedesmus* grows between 10 ˚C and 30˚C, dying out completely at 38˚C. Because the selected photobioreactor is closed, however, other conditions such as air particulate matter and humidity are minimally significant and assumed to be a non-issue for the process. The cultivation further requires inputs that are generated from other plants, namely ADC and flue gas. Thus, the optimization of location involved the range of temperatures throughout the year as well as proximity to both a wastewater treatment plant and a power plant. Factoring in the cost of land, the last limiting factor is the amount of space necessary (250 acres).

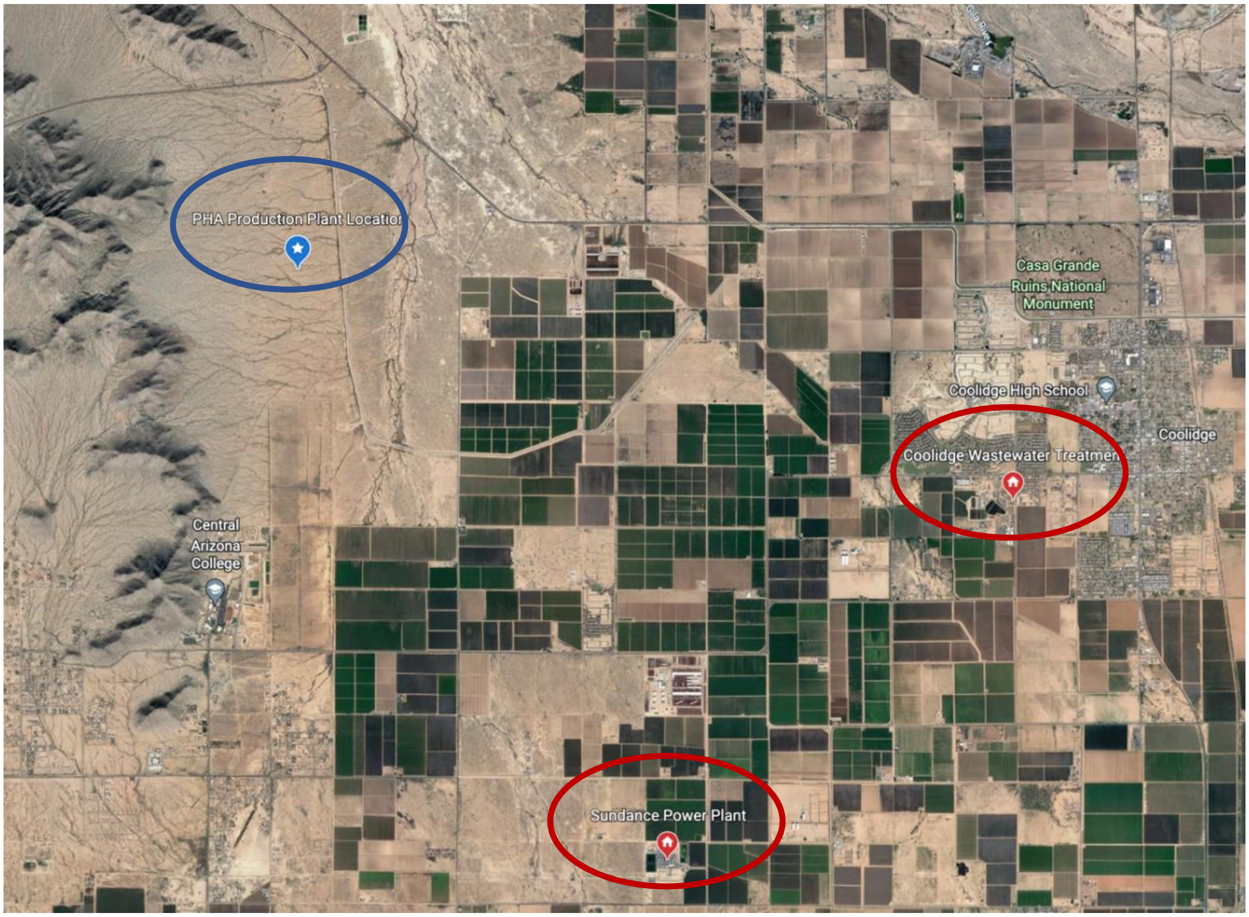
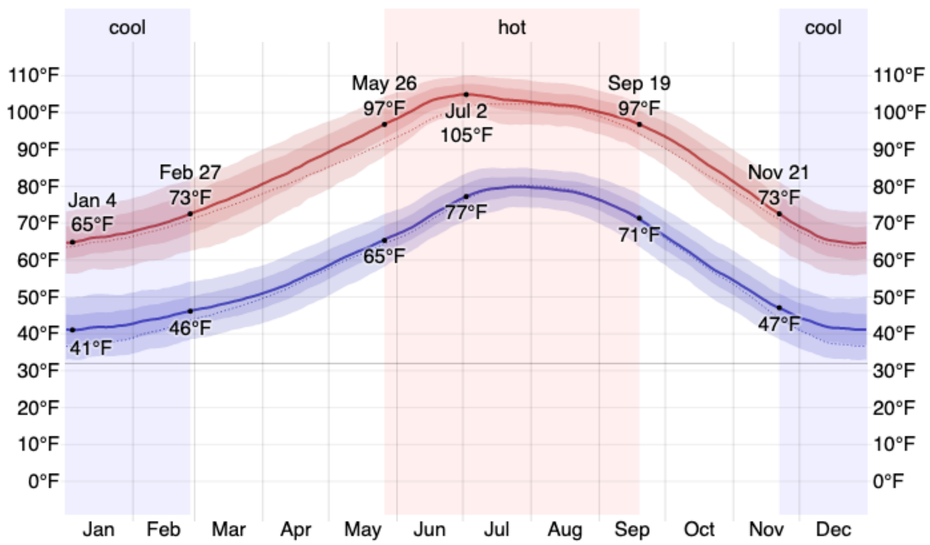


Figure 7. Aerial View of the Selected Location (Blue) and Related Plants (Red) in Coolidge, Arizona *(Google Earth)*

With all these factors considered, a plot of land in Coolidge, Arizona was selected as the plant location, shown in Figure 7. Both the Coolidge Wastewater Treatment Plant and Sundance Power Plant (natural gas) are located 10 miles from the selected location. The production rate of the wastewater treatment plant is more than sufficient for the needs of this process, and it is assumed that the ADC will be constantly pumped through a constructed pipeline (with no financial assistance from our plant) to the cultivation fields. Furthermore, it is assumed that desulfurization of flue gas occurs at the power plant, so the processed flue gas will be pumped through a constructed pipeline to a storage tank near the cultivation fields.

Coolidge, Arizona has temperatures that range from 5 ˚C to 40.5 ˚C on average, so to ensure that the algae remain at temperatures conducive to growth, temperature will be monitored and controlled with an internal heat exchanger. Figure 8 illustrates the range of temperatures as a monthly average across the course of a typical year (WeatherSpark, 2021)



Average	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
High	66°F	70°F	77°F	85°F	94°F	103°F	104°F	102°F	97°F	87°F	75°F	66°F
Temp.	53°F	56°F	62°F	70°F	79°F	89°F	92°F	90°F	85°F	73°F	60°F	52°F
Low	42°F	45°F	49°F	55°F	63°F	72°F	79°F	78°F	72°F	60°F	49°F	42°F

Figure 8. Average, High, and Low Daily Temperature in Coolidge, Arizona *(WeatherSpark, 2021)*

Plant Layout

100 hectares of land were deemed sufficient for algal cultivation (Fasaei et. al., 2018). This was split into 10 fields of 10 hectares each, with dimensions of 250 meters by 400 meters for maximum PBR volume. One inoculum system is required in total (3,000 m^2).

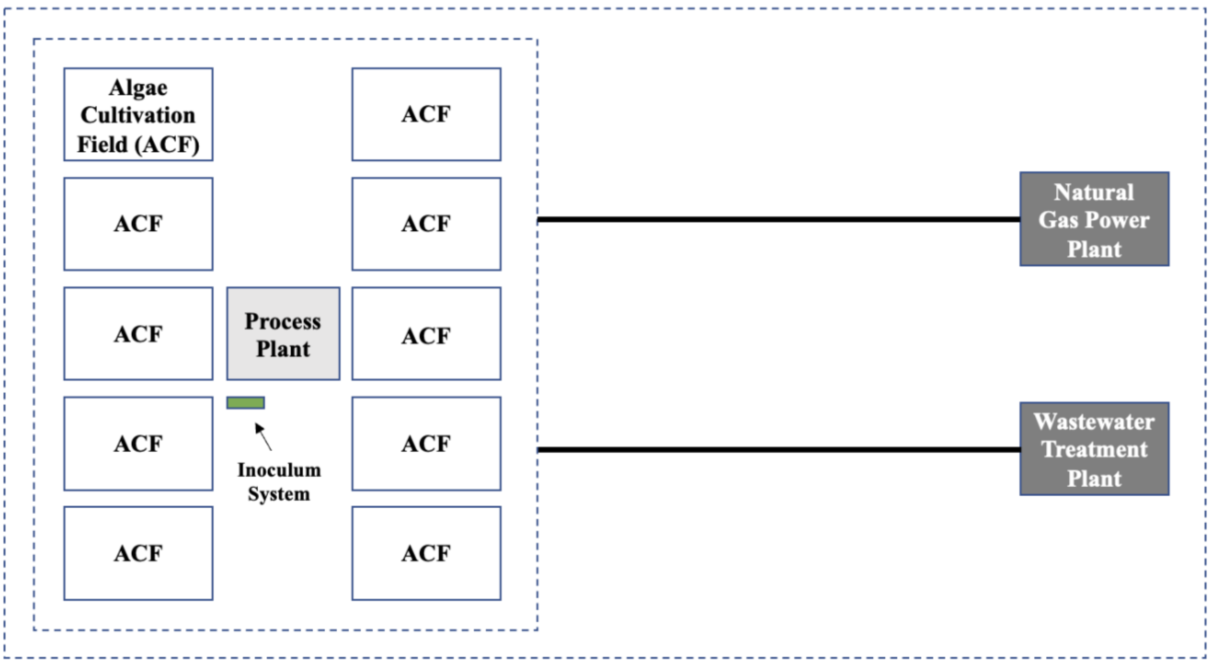


Figure 9. Aerial View of Plant Layout

As shown in Figure 9, the placement of the 10 algae cultivation fields is so that they are in proximity to the central process plant and the inoculum system. Each algae cultivation field needs access to the algae inoculant from the inoculum systems, and liquid must be transported between each field and the process plant. Outside the battery limits of the plant, pipelines 16,000 meters long (10 miles) are necessary for transportation of flue gas and ADC to the cultivation fields.

Assembly of Database

ASPEN Plus Modeling

ASPEN Plus is a powerful tool for modeling chemical engineering processes, but because of the difficulty in modeling chain polymers such as PHA and the inclusion of niche machinery such as photobioreactors and microbubble extraction units, ASPEN was used primarily for modeling two distillation columns at the end of our separation train. RADFRAC blocks were used to model the distillation of methanol from water and the distillation of chloroform from triolein. Design specifications were utilized to minimize the capital costs of the columns while also balancing the operating costs associated with the reboiler and condenser of each column. Unlike PHA, all four of these compounds were built into the ASPEN material database, so typical activity coefficient models such as UNIFAC and SRK were sufficient for modeling the binary interactions.

PHA Properties

As mentioned previously, this process assumes that a large majority of the PHA produced is PH3B, which has specific properties that can be used to characterize and identify the product produced, while also ensuring that the process does not exceed material property thresholds. For example, the glass transition temperature is 2˚C, which is important when considering the transport of PHA in cold ambient environments. Furthermore, the melting temperature is 179˚C, Young's Modulus is 3.5GPa, the tensile strength is 40 MPa, and the elongation to break is 5% (Jacquel et. al., 2007). Many of these properties are also useful when exploring the potential markets and applications for the specific kind of PHA produced in this process.

Raw Material Costs

The cost of each material was determined using several different sources. The costs for the two raw materials paid for in the process are listed in Table 2 below. The cost of methanol was found from Yadav et al., 2021. The cost of chloroform was found from a global chemical industry B2B website (ECHEMI, 2022). The costs of flue gas and ADC are assumed to be zero, as they are waste streams from their respective plants. Our project would provide cost savings for both plants by eliminating costs associated with disposal.

Table 2. Raw Material Costs for Process

Material	Cost	Units
Methanol	$0.44	1 kg
Chloroform	$0.94	1 kg

Process Flow Diagram and Material Balances

The process flow diagrams included in the figures below show the proposed process for the accumulation and isolation of PHA. The original block diagram accounted for algae cultivation, algae dewatering, PHA extraction, and PHA purification. Figure 10 shows an early-stage block flow diagram as a representation of our process before additional defining decisions were made.

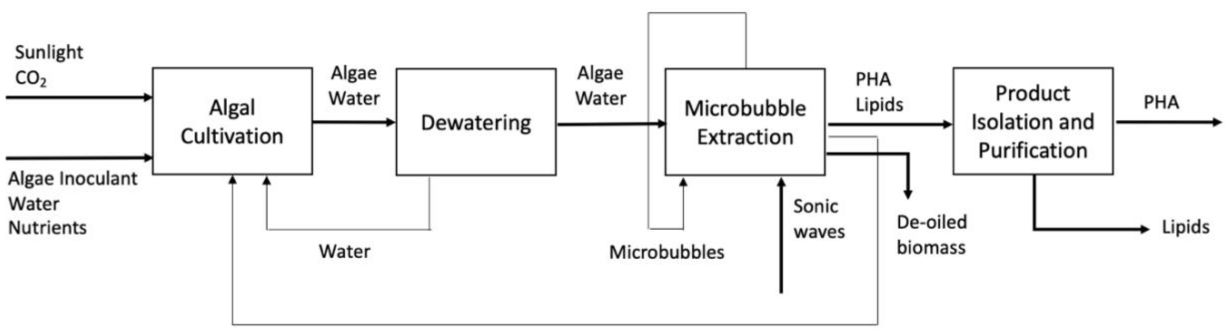


Figure 10. Preliminary Block Flow Diagram

Figures 11 and 12 illustrate the algae cultivation portion of the process, with a detailed account of a flat plate photobioreactor unit. Figure 13 shows the dewatering and extraction part of the process, in which DMB is isolated as a byproduct. Figure 14 shows the final separation portion of the process in which the PHA final product is separated from the lipid byproduct.

Flat Plate Photobioreactor Unit Diagram

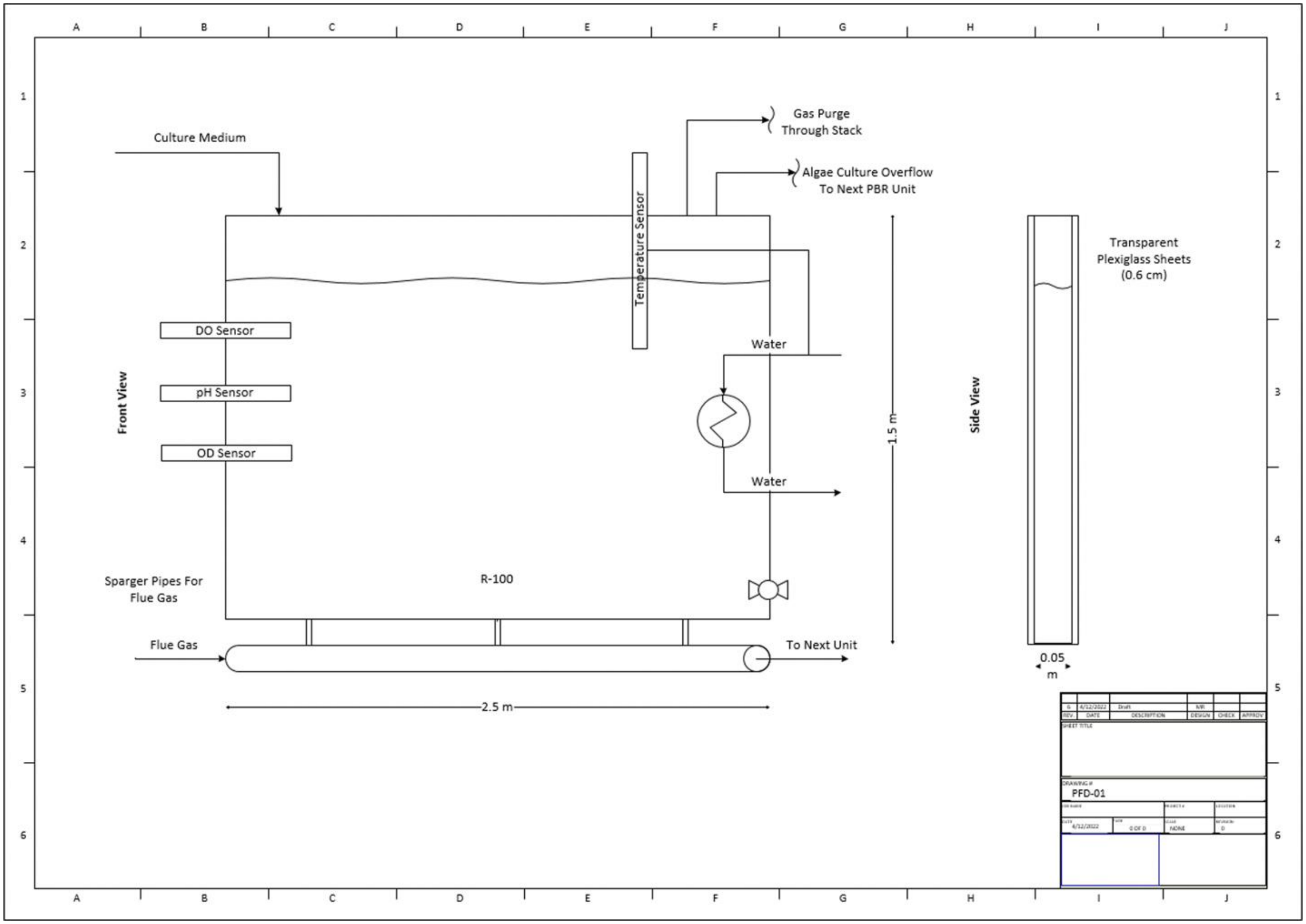


Figure 11. Flat Plate Photobioreactor Design (R-100)

Algae Cultivation Process Diagram

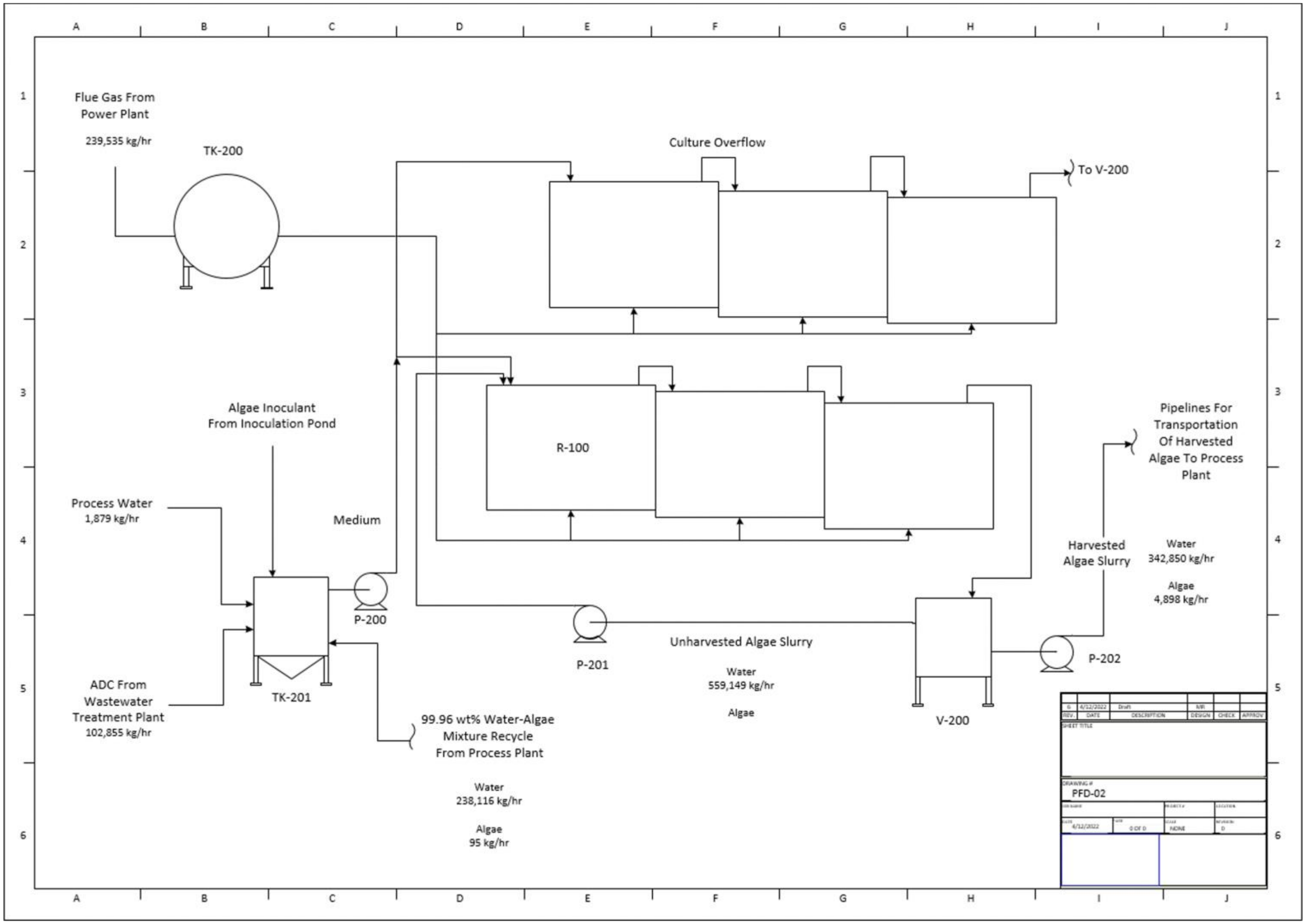


Figure 12. Process Flow Diagram for Algae Cultivation

Dewatering and Extraction Process Diagram

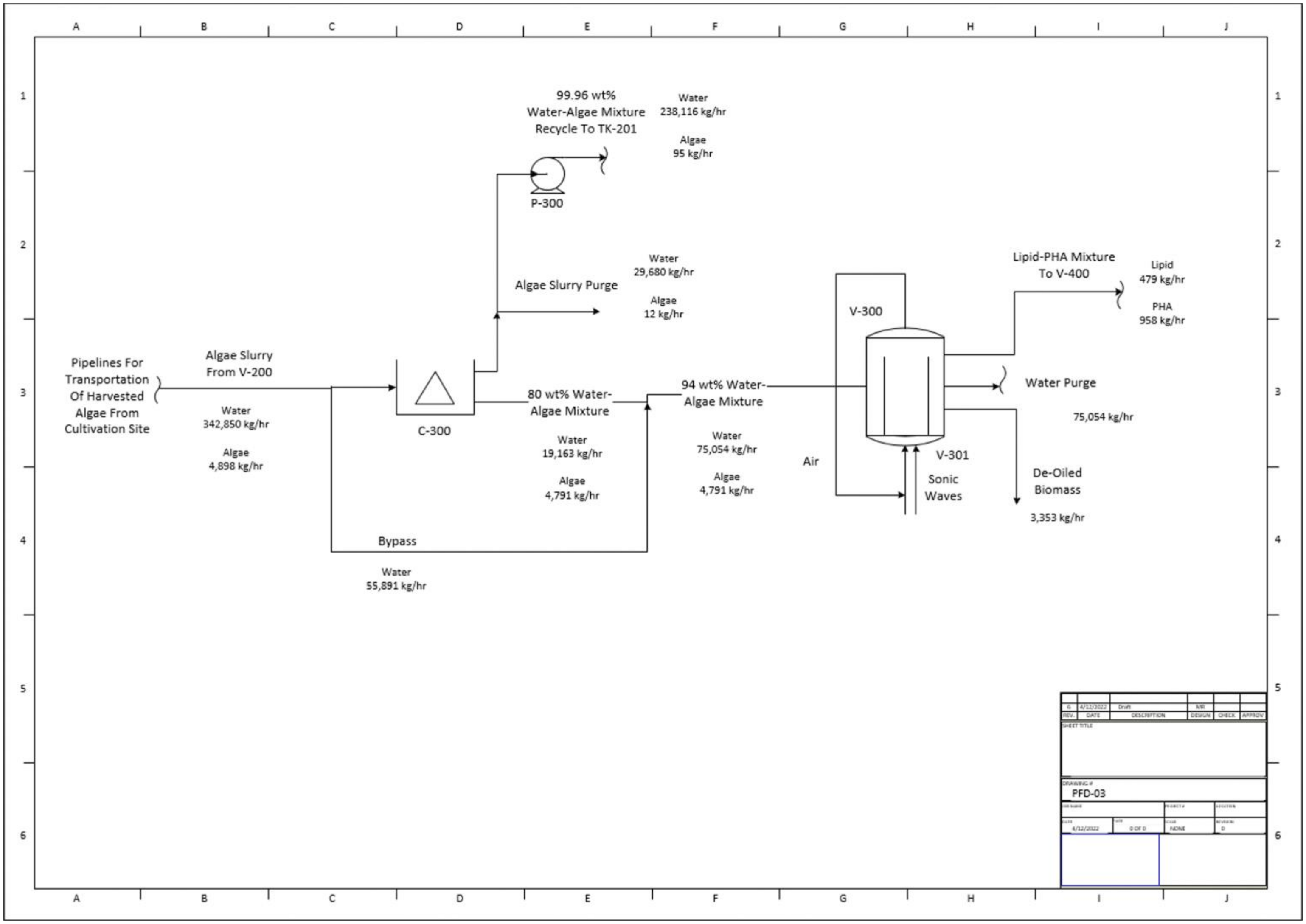


Figure 13. Process Flow Diagram for Dewatering and Extraction

Separation Process Diagram

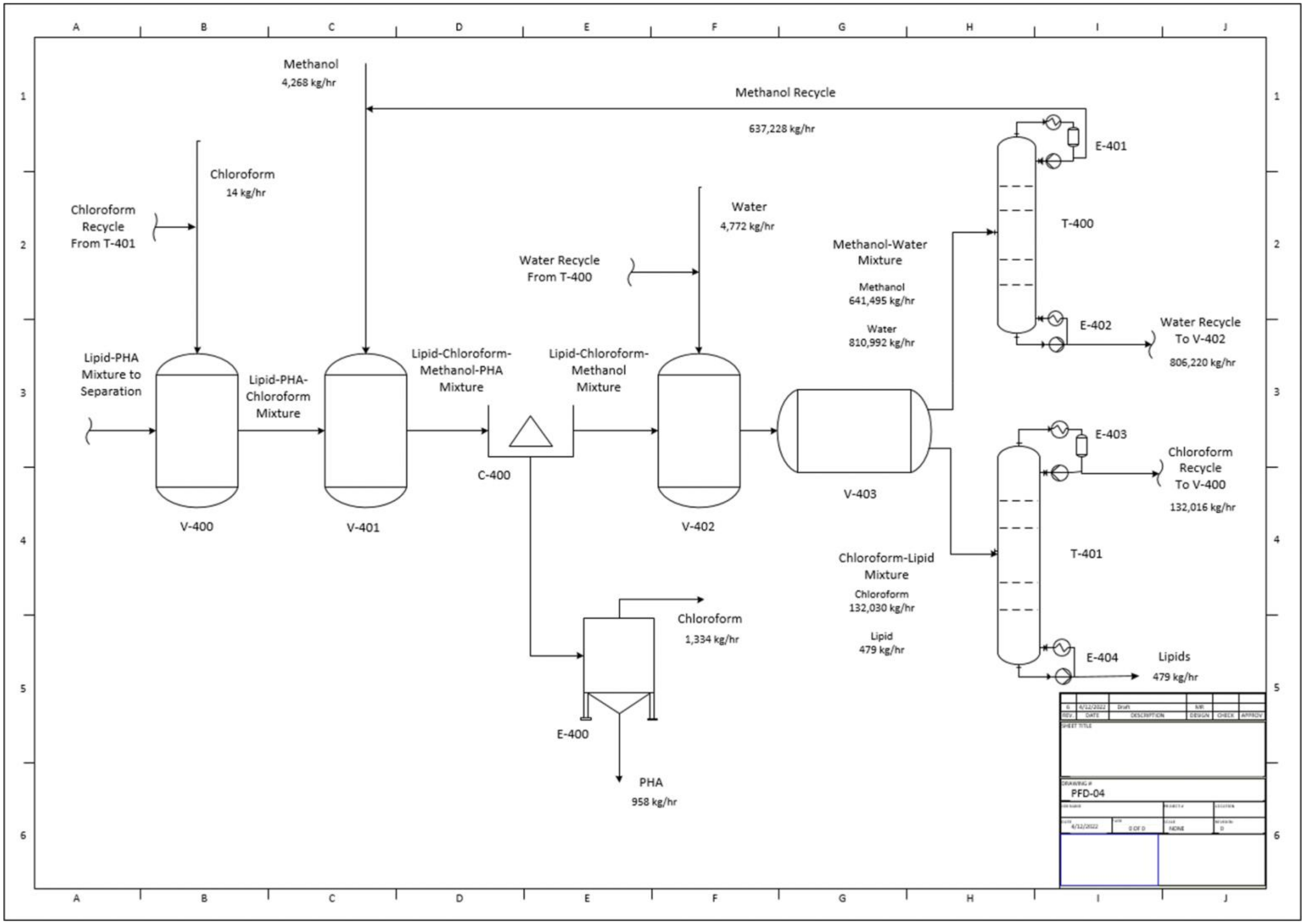


Figure 14. Process Flow Diagram for Separation

Process Description

This section will include narrative descriptions of the equipment chosen and function of each major piece of equipment. The reasons for the selection of these various pieces of equipment can be found above in the "Preliminary Process Synthesis" section.

Algal Cultivation

Culture Initiation

An inoculum system made of tubular photobioreactors is necessary to provide algae inoculant to the medium that is fed to the main culture, but a steady flow of this inoculant is not necessary. Instead, culture inoculation is simply needed for the initiation of culture, which is quantified by the dilution rate. This rate was chosen to be 0.33 $days^{-1}$ such that the plant harvests and replaces the total volume in the photobioreactors every 3 days (del Mar Morales-Amaral, 2015). This replaced medium is comprised of process water, algae inoculant, and ADC. Note that these three are first mixed in the medium preparation tank (TK-201) along with a recycled algae slurry from the dewatering centrifuge (C-300). Meanwhile, the recycled algae-water mixture from the gravity settler/bottom collection tank (V-200) is directly fed into the photobioreactors (R-100).

Photobioreactor

The selected flat panel photobioreactor (R-100), shown in Figure 11 above, will be vertical and in an east/west orientation in order to maximize sunlight. Several different materials are used for the transparent panes of the flat plate photobioreactors, mainly polyethylene, PVC, PMMA, glass, and Plexiglass. Borosilicate glass and PMMA (Plexiglas) proved superior due to their longer lifespans, productivity, light transmission, and ease of maintenance compared to plastic options including PE bags and PVC (SCHOTT, n.d.). When PE bags were used, the PBR bag replacement accounted for 31.4% of the plant's operating costs (Zhu, 2018).

After comparing glass and Plexiglas, the material selected for the flat plate photobioreactors is Plexiglas, otherwise known as Perspex, due to their similar lifespans and properties and the lower overall cost of Plexiglas (Tamburic, 2011). These panes will be 0.6 cm thick on either side of each unit (Khadim, 2018).

The optimal thickness between plates varies greatly, mostly between 2 to 7 cm. 5 cm was selected in order to optimize both light exposure and productivity (Masojidek & Torzillo, 2008) (Marsullo et. al., 2015). It is desirable for the volume of a PBR to be small because a thin optical thickness is helpful for light transfer (Huang Q. , 2017). A 2.5-meter length for each unit is considered standard (Sierra, et al., 2008).

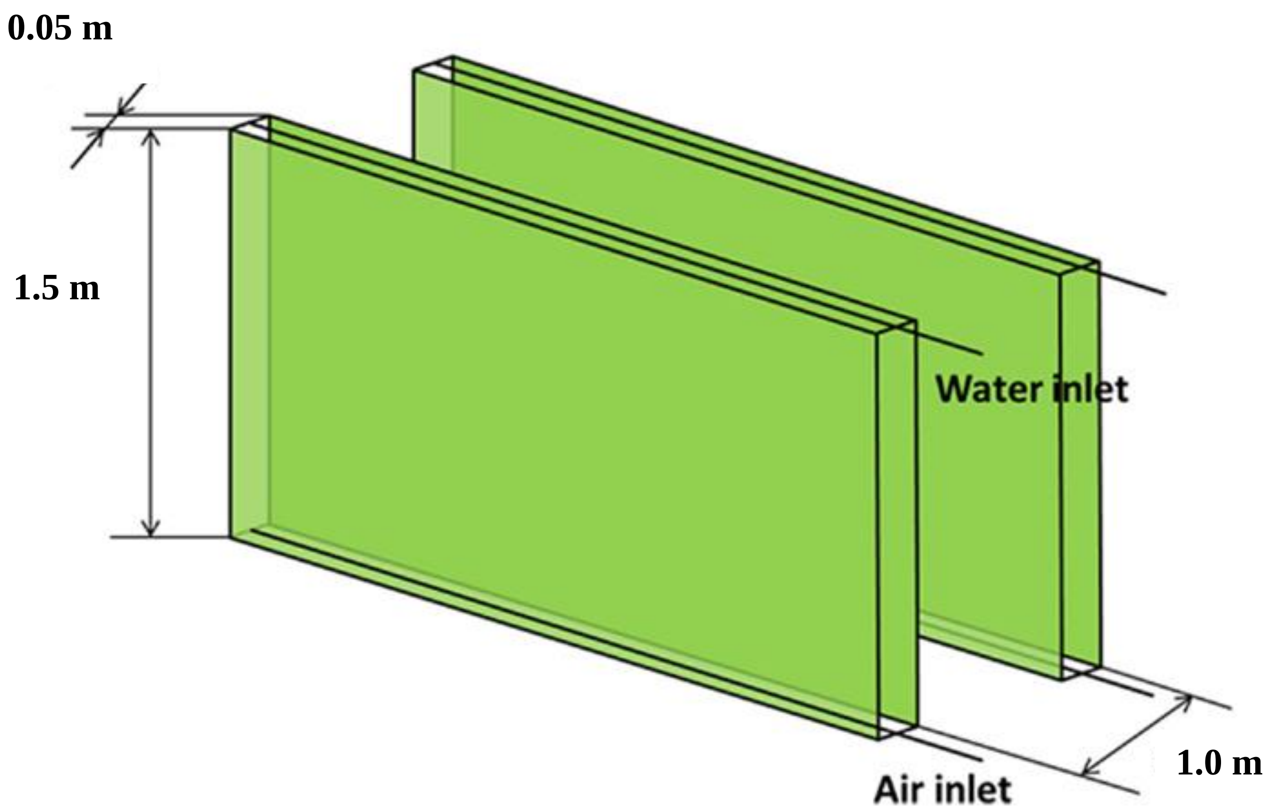


Figure 15. Specifications for Flat Plate Photobioreactor

Figure 15 shows a flat plate photobioreactor unit with specifications (Marsullo, et al., 2015). The reactor rows are spaced 1.0 meters apart in order to ensure that each pane gets adequate sun exposure.

Storage Tanks

After transportation of ADC from the wastewater treatment plant and flue gas from the natural gas power plant, the flue gas is kept in a storage tank (TK-200). This is placed near the inoculum system, as shown in Figure 9. The gas holder tank for flue gas is necessary so that it can be sparged as necessary according to the pH levels in the PBRs. The flue gas is fed into sparger pipes when alerted by the pH sensors.

The process water and ADC are fed directly into the medium preparation tank (TK-201) for mixing due to the continuous nature of the cultivation process. A cone roof storage tank was selected because open tanks may be subject to contamination from the outside environment, which is not ideal for algae cultivation purposes, and floating roof tanks are only necessary when a significant evaporation rate is expected (Seider et. al., 2017).

Algae inoculant and recycled water from the dewatering centrifuge (C-300) in the central process plant are also mixed in TK-201 along with the water and ADC before the medium is fed to the reactors (R-100). Feed pumps (P-200) distribute the medium to each photobioreactor row.

System Design

There are 10 separate fields for algae cultivation. Each field is each 100,000 m^2 (250 m x 400 m). There are 228 rows in each field with 1 m between rows and 10 m on the edge of each field for harvesting. Each row acts as one reactor with 156 units. The land is graded at 1%, which results in a 0.9° angle, causing algae culture to overflow from one unit to the next, with tanks at 97.4% of total volume. Figure 12 is a scaled-down example of one field, with only 2 rows and 3 units per row shown.

Each photobioreactor row functions as one reactor with multiple units. A pH sensor, OD measurement device (laser), and DO (dissolved oxygen) sensor are necessary to regulate the system (Skjanes, 2016; Salim, 2009) (Zhang, 2015). These sensors are placed every 10 units in order to identify trends in nutrient depletion and productivity while also saving costs per photobioreactor unit.

pH sensors are used as a proxy to measure the dissolved CO_2/carbonate levels to determine when more CO_2 is necessary to maintain optimal algae growth. In general, microalgae cultivation can occur in the pH range of 7 to 9 (Huang Q. , 2017). CO_2-rich flue gas is injected from the bottom of the PBRs from sparger pipes (Acien F. , 2012). This also has a mixing effect, known as airlift, which means that the contents of the bioreactor are agitated using gas (Cuello, 2016).

DO sensors are necessary because much of the dissolved oxygen released as a byproduct of photosynthesis is accumulated in the culture, which can reach a toxic level that may impact the survival of the microalgae (Huang Q. , 2017). Thus, a gas purge is necessary, and DO sensors help to regulate the frequency of such purges.

One temperature sensor is placed in the middle of each row in order to regulate the heat exchangers. The heat exchangers are small tubes which will be pumped full of cooling water or heating water depending on the surrounding temperature. This will not be necessary on most days of the year but is important to ensure the survival of the algae, as discussed above in the "Plant" section. Cooling water is necessary on approximately 88 days of the year. Heating water was neglected due to the infrequency of days in which the temperature goes below the lower limit. Cell death is also infrequent at low temperatures; it simply slows the growth of the algae. Additionally, the productivity rate taken was an average of productivity levels throughout the year (Clippinger & Davis, 2019).

There is a ball valve on the lowest unit for cleaning purposes. Unscrewing the valve will allow all the liquid to be released from the photobioreactor.

<u>Transportation of Materials</u>

Pipelines are used to transport ADC, flue gas, and process water from outside of the plant limits. Pipelines are also used to transport recycled water-algae slurry, recycled water, and recycled solvent within the plant. Pumps (P-202 and P-300) are necessary for the pipeline transportation.

Production Rate

The productivity of the PBRs was determined by looking at several sources for algae cultivation in flat panel PBRs of various depths, with some using Scenedesmus and others not. 1.81 g/L/day was deemed reasonable for the volumetric productivity of the flat plate PBR system (Clippinger & Davis, 2019). This number was sourced directly from a paper by the National Renewable Energy Laboratory, but other sources corroborate this as a fitting estimate (de Vree, 2015) (Barbera, 2015) (Koller, 2018). A volumetric basis is a more standard productivity measure than areal productivity, which may represent either reactor surface area or land area.

Harvesting and Dewatering

Each field has seven bottom collection tanks (V-200), so each set of 32 to 33 rows shares a tank with a collective stream in for algae from the PBRs. In this tank, the primary dewatering occurs via gravity settling occurs, resulting in a stream of concentrated algae and one of mostly water recirculated to main cultivation. An algae concentration of 10 g/L is assumed post-gravity settling for the harvested algae slurry.

The unharvested algae slurry is returned directly to the PBRs (R-100) instead of the medium preparation tanks, as the slurry is assumed to be the proper concentration for the photobioreactors and requires no mixing. Note, however, that ADC flow rates are not considered after the algae cultivation stage. In this study, ADC is treated as nutrient-enriched water, and since the nutrients are assumed to have been consumed by the algae by primary dewatering, all remaining liquid is treated as water.

After the algae-water mixture has settled to a concentration of 10 g/L, this concentrated mixture of harvested algae is transported from the cultivation fields and pumped (P-202) into a bowl centrifuge (C-300), which can concentrate the algae slurry to 80 wt% water, with a recycle stream back to the main photobioreactors at a concentration of 99.96 wt% (assuming a dewatering efficiency of 97%) (Davis, et al., 2016). Since the extraction unit (V-300) only requires a water weight percent of 94%, a bypass stream of water is taken around the centrifuge to minimize the size, and thus capital cost, required for the centrifugation system.

Microbubble Extraction

Scaling the results of the study conducted by Yadav, the input of the extraction unit is 93.9 wt% water. From the bottom of the unit, 20,000 microbubbles per second are injected for the lysing of the algae cell walls (Yadav, et al., 2021). Ultrasonic disruption should occur with continuous low frequency waves at 0.6 MHz and microbubbles of an average radius of 50 microns (Land, Unpublished, 2022). The extractor should be operated at atmospheric pressure. Despite the operation of the extraction vessels at 5.0 MMPa in Yadav, et al (2021), this high of a pressure was deemed unnecessary (Land, Unpublished, 2022). For biodiesel production, the extractor (V-300) is set at 95 °C. However, for the purposes of PHA isolation, ambient temperature was considered appropriate. It is assumed that all the biomass is able to exit the extraction cylinder and move into the outer cylinder.

In this outer cylinder (V-301), gravity settling will occur. The gravity settler is expected to separate the resulting flow from the extraction process into several layers: a lipid-PHA layer at the top, followed by a layer of water, and the de-oiled biomass at the bottom (Yadav et. al., 2021). These streams will all be removed separately, with de-oiled biomass removed to be sold as a byproduct, water recycled forward to the separation process, and the lipid-PHA mixture continuing to the separation process.

Composition varies depending on culture conditions. For example, nitrogen limitation and high light conditions yields more lipid and less carbohydrate (Yousuf, 2020). The weight of PHA and lipids out of total biomass weight, 20% and 10% respectively, were assumed (Garcia, et al., 2021) (Grima, 2003), leaving a remainder of 70% for de-oiled biomass, which consists of carbohydrates, proteins, pigments, and nucleic acids. These numbers were determined by performing a linear interpolation with the production data from Garcia, et al. (2021).

Separation

In the first agitated vessel (V-400), chloroform is added so that maximum solubility of chloroform can be assumed for both PHA and triolein (National Library of Medicine, 2022) (See Appendix). In the second agitated vessel (V-401), methanol is added in a 9:1 ratio to the existing chloroform, which then precipitates out the PHA (Salim, 2009). It is assumed that this slurry with PHA solid is able to flow to the centrifuge (C-400), and that the PHA is not sticky.

From the centrifuge (C-400), it is assumed that the PHA comes out with 1% of the original chloroform. This outlet stream goes to an evaporator to dry the PHA at 60 C (Salim, 2009). There is a favorable interaction that helps binds the chloroform to the PHA. It is assumed that we are just evaporating chloroform and no interaction is occurring.

The other outlet stream from C-400 goes on to the third agitated vessel, where water is added in a 1:1 ratio with methanol. As shown in Figure 6, this is necessary in order to create two phases. This mixture flows into the next vessel, a decanter (V-402), where it is assumed that the two phases fully separate. From there, the methanol-water mixture enters a distillation column (T-400) and the triolein-chloroform mixture enters another distillation column (T-401). Four distillation columns are necessary to handle the large volume of liquid present. The methanol and water streams exiting T-400 are recycled to vessels V-401 and V-402 respectively. The chloroform stream exiting T-401 is recycled to V-400, and the triolein is sold as a byproduct.

Energy Balance and Utility Requirements

The heat exchangers for the photobioreactor, as well as the condensers and reboilers for the distillation columns, had various energy demands for heating and cooling. Positive heat duties are associated with heating requirements, and negative neat duties are associated with cooling requirements. The heat duties of individual pieces of equipment are detailed in Table 3.

Table 3. Energy Demands of Equipment

Equipment ID	Equipment Description	Heat Duty (kW)
R-100	Flat-Plate Photobioreactors	-634.99
E-401	Methanol-Water Distillation Column Condenser	-396054
E-402	Methanol-Water Distillation Column Reboiler	492552
E-403	Triolein-Chloroform Distillation Column Condenser	-16235.8
E-404	Triolein-Chloroform Distillation Column Reboiler	17630.9

In order to meet the energy demands listed above in Table 3, utilities are necessary for heating (high pressure steam) and cooling (cooling water). Process water is also required for this process. Quantities of utilities required by equipment and corresponding costs are listed in Table 4. The costs of utilities were referenced from Seider et al, 2017. After pulling the heat duties for the reboilers and condensers from ASPEN, the flow rates for the steam were determined based on the latent heat of vaporization, while the flow rates for the cooling water were determined based on a $\Delta T = 16.7^{\circ}C$ as the water temperature increases from 90 to 120˚F. These flow rates were then scaled up to an annual basis and converted to a cost.

Table 4. Quantities and Costs of Utilities Required

Cooling Water			
Equipment ID	**Quantity (gal/hr)**	**Quantity (gal/yr)**	**Annual Cost ($/yr)**
R-100	2,146	67,998,405	6,958
E-401	5,363,550	42,479,319,735	$4,247,932
E-403	219,873	1,741,391,433	$174,139
High Pressure Steam			
Equipment ID	**Quantity (lb/hr)**	**Quantity (lb/yr)**	**Annual Cost ($/yr)**
E-402	173,233	1,372,008,506	$10,976,068
E-404	62,009	491,110,477	$3,928,884
Process Water			
Equipment ID	**Quantity (kg/hr)**	**Quantity (kg/yr)**	**Annual Cost ($/yr)**
R-100, V-402	6,651	52,678,492	$11,119

In addition to the utility requirements, additional operating costs are accumulated by electricity requirements. Electricity was needed to run the pumps, centrifuges, and agitators in this process. Power required by equipment and corresponding costs are listed in Table 5. $0.07/kW-hr was used as the price of electricity (Seider, et al., 2017). The electricity usage for the pumps and agitators (in the vessels) were calculated from the power needed (converted from Hp to kW and then scaled up to an annual scale). The evaporator was based on the latent heat of chloroform (247 kJ/kg) and the amount of chloroform still present with the PHA (1% of the original).

Table 5. Quantities and Costs of Electricity Required

Equipment ID	Equipment Description	Power Requirement (kW)	Annual Energy Usage (kW-yr)	Annual Cost ($/yr)
P-200	Feed Pumps to Photobioreactor	559.4	4,430,448	$310,131
P-201	Algae Recirculation Pump	3915	31,006,800	$2,170,476
P-202	Harvested Algae Pump	559.3	4,429,656	$310,076
C-300	Centrifuge for Algae Dewatering[a]	-	-	$2,713,684
P-300	Pump for Recycle to Cultivation	55.9	442,728	$30,991
P-301	Pump to Extraction Vessel	1081	8,561,520	$599,306
V-400	Vessel for Chloroform Addition	4.56	36,092	$2,526
V-401	Vessel for Methanol Addition	25.67	203,294	$14,231
C-400	Centrifuge for PHA Removal[a]	-	-	$7,341,203
E-400	Evaporator for PHA Drying	91.50	724,695	$50,729
V-402	Vessel for Water Addition	52.33	414,475	$29,013

[a]Centrifuges were priced based on a proprietary design (scaled relative to feed flow rates) in Davis et. al., 2017.

Equipment List and Unit Descriptions

Table 66. Summary of Equipment Identifiers and Descriptions

Equipment ID	Equipment Description
R-100	Flat plate photobioreactors

TK-200	Storage tank for flue gas
TK-201	Medium preparation tank
P-200	Feed pumps to algae cultivation
V-200	Gravity settler for harvesting
P-201	Algae recirculation pump
P-202	Harvest pump
C-300	Centrifuge for dewatering
P-300	Algae recycle pump to cultivation
V-300	Extraction vessel
V-301	Gravity settler
V-400	Vessel for chloroform addition
V-401	Vessel for methanol addition
C-400	Centrifuge for PHA isolation
E-400	Evaporator for PHA drying
V-402	Vessel for water addition
V-403	Decanter
T-400	M/W distillation column
E-401	Condenser on M/W distillation column
E-402	Reboiler on M/W distillation column
T-401	Lipid/chloroform distillation column
E-403	Condenser on L/C distillation column
E-404	Reboiler on L/C distillation column

Reactors

R-100

The flat plate photobioreactors are necessary to cultivate the algae. Each unit is 1.5 meters tall and 2.5 meters long, with a spacing of 0.05 m between plates. The plates are made of Plexiglas, 0.6 cm thick. Each reactor has 156 units. Each field has 228 rows, each of which functions as one reactor. The inputs to the flat plate PBRs are the medium feed from the preparation tank (TK-201) and the algae slurry recycle from the bottom circulation tank (V-200). The medium flow rate from TK-201 is equivalent to the flow rate that leaves the cultivation fields as the harvested algae stream.

Within the reactor units, small tubes act as a heat exchanger for temperature control. 67,998,405 gal/yr of cooling water are necessary. The DO (dissolved oxygen) sensor manages gas purge to avoid oxygen buildup. The pH sensor manages flue gas (CO_2) injection and purge. The OD (optical density) sensor measures cell growth. A ball valve on last unit is used for reactor wash out.

Storage Tanks

TK-200

The sparging of flue gas is regulated by the pH sensors, so a storage tank is needed to store the incoming flue gas before it is deemed necessary to distribute it to the photobioreactors. The flue gas arrives in pipelines from a natural gas power plant. This gas holder storage tank, constructed out of carbon steel, is at ambient temperature and pressure with a capacity of 1,593.7 m^3. This tank is able to hold 30-minutes' worth of flue gas, so it can be sparged as alerted by the pH sensors when more CO_2 is necessary for algae cultivation.

TK-201

The medium preparation tank is where the process water, anaerobic digestion centrate (ADC), recycled algae from the central process plant, and algae inoculant from the inoculum system are mixed before being fed to the photobioreactors. This cone roof storage tank, constructed out of carbon steel, is at ambient temperature and pressure with a capacity of 90.2 m^3. Algae inoculant is only fed if the culture crashes and the plant has excessive downtime.

Pumps

Note that all the pumps in this system are constructed from stainless steel. In most cases, the inlet and outlet pressures are not known precisely because ASPEN cannot be used to model the pipe flow and corresponding pressure drops. A heuristic was used from Seider et al. (2017) to determine the heads for each pump: For liquid flow, a pipeline pressure drop of 2 psi was assumed for every 100 feet of pipe. For each 10-foot rise in elevation, a pressure drop of 4 psi was assumed.

P-200

Centrifugal pumps are used in each field to pump the culture medium from the medium preparation tanks (TK-203) into the photobioreactors (R-100). The flow rate is 148.6 gal/min and the head is 7.6 ft. It has a shaft RPM of 3,600 and a VSC orientation. The electricity requirement is 559.4 kW.

P-201

These centrifugal pumps recirculate unharvested algae from the gravity settler (V-200) to the medium preparation tanks (TK-201). An average pipe length of 250 meters was accounted for in the calculation of pressure drop. The flow rate is 34.6 gal/min and the head is 60.6 ft. It has a shaft RPM of 3,600 and a VSC orientation. The electricity requirement is 3915.0 kW.

P-202

These centrifugal pumps transport the harvested algae from the cultivation fields to the process plant. This allows the harvested algae to be fed to the centrifuge (C-300). An average pipe length of 400 meters was accounted for in the calculation of pressure drop. The flow rate is 150.7 gal/min and the head is 37.9 ft. It has a shaft RPM of 3,600 and a VSC orientation. The electricity requirement is 559.3 kW.

P-300

These centrifugal pumps return the remaining algae slurry (99.96 wt% water-algae mixture) to medium preparation tanks (TK-202) for re-entry into the photobioreactors. An average pipe length of 400 meters was accounted for in the calculation of pressure drop. The flow rate is 103.2 gal/min and the head is 37.9 ft. It has a shaft RPM of 3,600 and a VSC orientation. The electricity requirement is 55.9 kW.

Pressure Vessels

Note that all the pressure vessels in this system were constructed from 304 stainless steel.

V-200

The function of the gravity settler at the algae cultivation site is for algae harvesting. Here, a concentrated algae slurry of 10 g/L settles to the bottom of the tank, where it is harvested for transport to the main process plant. The unconcentrated algae slurry at the top of the tank is recirculated to the medium preparation tank (TK-203). This vessel is at ambient temperature and pressure with a capacity of 76.3 m^3.

V-300

The purpose of this vessel is for cell lysis to take place. This vessel is operated at atmospheric temperature and pressure. Microbubbles from the bottom of the unit combined with ultrasonic waves produced by the sonicator work together to lyse the cells. Algae is fed to the vessel, and after lysis, PHA, lipids, and DMB flow to the outer cylinder. A residence time of 10 minutes was assumed, with a tank volume equivalent to the holdup volume in order to ensure overflow, and an aspect ratio (L/D) of 2.5. The radius of the vessel is 1.2 m, and the height is 6.1 m.

V-301

Liquid overflows from the extraction vessel (V-300) into this vessel. Complete overflow is assumed. The purpose of this vessel is gravity settling for the separation of the liquid into three streams: PHA-lipid mixture, water for recycle, and de-oiled biomass. A residence time of 10 minutes was assumed, with a tank volume of twice the holdup volume, and an aspect ratio (L/D) of 2.5. The radius of the vessel is 3.4 m, and the height is 16.8 m.

V-400

The purpose of this vessel is for chloroform addition in order to dissolve the PHA and lipid. A residence time of 10 minutes was assumed, with a tank volume of twice the holdup volume, and an aspect ratio (L/D) of 2. The radius of the vessel is 1.5 m, and the height is 6.2 m. An agitator (propellor) was necessary for agitation of the mixture and the solvent. This has an electricity requirement of 1.3 kW.

V-401

The purpose of this vessel is for methanol addition in order to precipitate out the PHA. Methanol is added in a 9:1 volume ratio with the chloroform added in V-400. A residence time of 10 minutes was assumed, with a tank volume of twice the holdup volume, and an aspect ratio (L/D) of 2. The radius of the vessel is 2.7 m, and the height is 11.0 m. An agitator (turbine) was necessary for agitation of the mixture and the solvent. This has an electricity requirement of 7.2 kW.

V-402

The purpose of this vessel is for water addition in order to create two separate phases: one for methanol and water and one for chloroform and lipid. Water is added in a 1:1 volume ratio with the methanol added in V-401. A residence time of 10 minutes was assumed, with a tank volume of twice the holdup volume, and an aspect ratio (L/D) of 2. The radius of the vessel is 3.5 m, and the height is 13.9 m. An agitator (turbine) was necessary to ensure that the mixture is well mixed. This has an electricity requirement of 14.6 kW.

V-403

The decanter is meant to create a quiet zone for the full separation into two phases before feeding the streams separately into distillation towers. A residence time of 10 minutes was assumed, with a tank volume of twice the holdup volume, and an aspect ratio (L/D) of 2. This is a horizontal vessel, with radius 3.5 m and length 13.9 m.

Centrifuges

C-300

The purpose of this bowl centrifuge, constructed from 304 stainless steel, is to act as the main dewatering step. It receives an algae slurry at 10 g/L (99 wt% water) after gravity settling occurs and its outputs are water-algae mixtures of 80 wt% for entrance to the extraction unit and 99.96 wt% for recycle to the cultivation fields. Since this centrifuge has the capability to reduce the water wt% to 80%, there is a bypass water stream that goes around the centrifuge because the extraction unit only requires 94 wt% water. Due to the volume of the recycle stream, a portion of it is purged so that some fresh process water can also be fed to the PBRs.

C-400

The purpose of this continuous reciprocating pusher centrifuge, constructed from 304 stainless steel, is to remove the precipitated PHA from the solution. 1% of the original volume of chloroform added comes out with the PHA. The remaining 99% of the chloroform, along with the full volumes of methanol and triolein, proceed to the next vessel.

Towers

Note that both towers are constructed from stainless steel, were designed at atmospheric pressure, and contain sieve trays.

T-400

The purpose of the distillation column is to separate the methanol and water so that they can be recycled. This column has a diameter of 8.6 m, and 30 equilibrium stages (height of 17.5 m). The condenser (E-401) has a heat duty of -396,054.4 kW and the reboiler (E-402) has a heat duty of 492,552.0 kW.

T-401

The purpose of the second distillation column is to separate the chloroform and lipid so that the chloroform can be recycled, and the lipid can be sold as a byproduct. This column has a diameter of 4.2 m, and 15 equilibrium stages (height of 10.7 m). The condenser (E-403) has a heat duty of -16,235.8 kW and the reboiler (E-404) has a heat duty of 17,630.9 kW.

Other

E-400

The purpose of the evaporator is to dry the PHA after centrifugation (C-400), removing residual chloroform, which was assumed to be 1% of the original input. The evaporator is a continuously operating unit, draft-tube baffled. It dries 25.4 tons of crystals per day, operating at 60 °C with a heat duty of 91.5 kW.

Sonicator

The purpose of the sonicator is to provide ultrasonic waves to the extraction vessel of 0.6 MHz to lyse the cells.

FTIR Spectroscopy Machine

The purpose of this machine is for product quality control. It will allow us to take samples of product to confirm which type of PHA is being produced.

Specification Sheets

Reactors

Flat Plate Photobioreactor			
Identification:	**Item**	R-100	
	No. Req	2,330	
Function:	Algae cultivation		
Operation:	Continuous		
Materials Handled:			
	Inlet 1	Inlet 2	Outlet
Temperature (°C)	25	25	25
Pressure (atm)	1	1	1
Component Mass Flow (kg/hr)			
Algae	96	*	4,898*
Water	239,995	559,149	342,850
ADC	102,855	**	**
Design Data:			
	Height (m)	1.5	
	Width (m)	2.5	
	Material of Construction	Plexiglas	
Utilities:	Cooling water: 67,998,405 gal/yr		
Total Purchase Cost		$35,607,679	
Total Bare Module Cost		$81,897,662	
Comments: *The unharvested algae flow rate varies and is recirculated directly back to the PBRs, so the algae material balance neutralizes in the outlet stream. **All liquid is assumed to be water after PBRs because nutrients are consumed from ADC.			

Storage Tanks

Storage Tank for Flue Gas			
Identification:	**Item**		TK-200
	No. Req		1
Function:	Storing the flue gas until the pH levels in the PBRs require more to be sparged		
Operation:	N/A		
Materials Handled:			
		Inlet	Outlet
Temperature (°C)		25	25
Pressure (atm)		1	1
Component Mass Flow (kg/hr)			
Flue Gas		239,535	239,535
Design Data:			
	Type		Gas Holder
	Volume (m^3)		1,593.7
	Material of Construction		Carbon Steel
Utilities: N/A			
Total Purchase Cost			$396,507
Total Bare Module Cost			$2,237,786
Comments: The flue gas flow rates are average values. This tank is designed to hold half-an-hours-worth of flue gas.			

Medium Preparation Tank				
Identification:	**Item**	TK-201		
	No. Req	10		
Function:	Mixing water, ADC, and recycled algae slurry before feeding the medium to the PBRs			
Operation:	N/A			
Materials Handled:				
	Inlet 1	Inlet 2	Inlet 3	Outlet
Temperature (°C)	25	25	25	25
Pressure (atm)	1	1	1	1
Component Mass Flow (kg/hr)				
Water	1,879	0	238,116	239,995
ADC	0	102,855	0	102,855
Algae	0	0	95	95
Design Data:				
	Type	Cone Roof		
	Volume (m^3)	90.2		
	Material of Construction	Carbon Steel		
Utilities:				
Total Purchase Cost		$297,755		
Total Bare Module Cost		$502,983		

Comments: Algae inoculant is added here when necessary to revive culture. Enough process water is added to fully replace the water in the medium every 2 weeks, with the recycle from the centrifuge purged accordingly.

Pumps

Feed Pumps to Photobioreactors		
Identification:	**Item**	P-200
	No. Req	10
Function:	Pumping the culture medium up into the photobioreactors	
Operation:	Continuous	
Materials Handled:		
	Inlet	Outlet
Temperature (°C)	25	25
Pressure (atm)	*	1
Component Mass Flow (kg/hr)		
Algae	4,898	4,898
Water	138,938	138,938
Design Data:		
	Type	Centrifugal
	Flow Rate (gal/min)	148.6
	Head (ft)	7.6
	Material of Construction	Stainless Steel
	Shaft RPM	3,600
	Case-Split Orientation	VSC
Utilities:	Electricity: 559.4 kW	
Total Purchase Cost		$88,810
Total Bare Module Cost		$413,507
Comments: *Account for the head as listed above		

Algae Recirculation Pump		
Identification:	**Item**	P-201
	No. Req	70
Function:	Pumping the unharvested algae slurry back to the medium preparation tank	
Operation:	Continuous	
Materials Handled:		
	Inlet	Outlet
Temperature (°C)	25	25
Pressure (atm)	*	1
Component Mass Flow (kg/hr)		
Algae	**	**
Medium	559,149	559,149
Design Data:		
	Type	Centrifugal
	Flow Rate (gal/min)	34.6
	Head (ft)	60.6
	Material of Construction	Stainless Steel
	Shaft RPM	3,600
	Case-Split Orientation	VSC
Utilities:	Electricity: 3915.0 kW	
Total Purchase Cost		$660,170
Total Bare Module Cost		$3,073,807

Comments: *Account for the pressure drop across the recirculation pipelines (see head); **The unharvested algae flow rate varies and is recirculated directly back to the PBRs, so the algae material balance neutralizes in the outlet stream.

Harvested Algae Pump		
Identification:	**Item**	P-202
	No. Req	10
Function:	Pumping the harvested algae slurry to the central process plant (into centrifuge)	
Operation:	Continuous	
Materials Handled:		
	Inlet	Outlet
Temperature (°C)	25	25
Pressure (atm)	*	1
Component Mass Flow (kg/hr)		
Algae	4,898	4,898
Water	342,850	342,850
Design Data:		
	Type	Centrifugal
	Flow Rate (gal/min)	150.7
	Head (ft)	37.9
	Material of Construction	Stainless Steel
	Shaft RPM	3,600
	Case-Split Orientation	VSC
Utilities:	Electricity: 559.3 kW	
Total Purchase Cost		$86,120
Total Bare Module Cost		$400,982
Comments: *Account for the pressure drop across the transportation pipelines (see head)		

Pump for Recycle to Cultivation		
Identification:	**Item**	P-300
	No. Req	1
Function:	Pumping the remaining 99.96 wt% water-algae mixture back to cultivation	
Operation:	Continuous	
Materials Handled:		
	Inlet	Outlet
Temperature (°C)	25	25
Pressure (atm)	*	1
Component mass flow (kg/hr)		
Algae	95	95
Water	238,116	238,116
Design Data:		
	Type	Centrifugal
	Flow Rate (gal/min)	103.2
	Head (ft)	37.9
	Material of Construction	Stainless Steel
	Shaft RPM	3,600
	Case-Split Orientation	VSC
Utilities:	Electricity: 55.9 kW	
Total Purchase Cost		$86,110
Total Bare Module Cost		$400,935
Comments: *Account for the pressure drop across the transportation pipelines (see head)		

Pressure Vessels

Bottom Circulation Tank			
Identification:	**Item**	V-200	
	No. Req	70	
Function:	Gravity settler for algae harvesting		
Operation:	Continuous		
Materials Handled:			
	Inlet	Outlet 1	Outlet 2
Temperature (°C)	25	25	25
Pressure (atm)	1	1	1
Component Mass Flow (kg/hr)			
Algae	4,898*	4,898	*
Medium	901,999	342,850	559,149
Design Data:			
	Volume (m^3)	76.3	
	Material of Construction	Carbon Steel	
	Design Pressure (atm)	1	
	Residence Time	10 minutes	
Utilities: N/A			
Total Purchase Cost		$396,423	
Total Bare Module Cost		$665,908	
Comments: *The unharvested algae flow rate varies and is recirculated directly back to the PBRs, so the algae material balance neutralizes in the outlet stream.			

Extraction Vessel		
Identification:	**Item**	V-300
	No. Req	1
Function:	Cell lysis for the removal of PHA and lipids	
Operation:	Continuous	
Materials Handled:		
	Inlet	Outlet
Temperature (°C)	25	25
Pressure (atm)	1	1
Component Mass Flow (kg/hr)		
Algae	4,791	0
Water	75,054	75,054
PHA	0	958
Lipids	0	479
De-Oiled Biomass	0	3,353
Design Data:		
	Height (m)	6.1
	Radius (m)	1.2
	Material of Construction	304 Stainless Steel
	Design Pressure (atm)	1
Utilities: N/A		
Total Purchase Cost		$97,861
Total Bare Module Cost		$574,399
Comments:		

Gravity Settling Vessel					
Identification:	**Item**		V-301		
	No. Req		1		
Function:	Separation of the PHA-lipid mixture, de-oiled biomass, and water after cell lysis				
Operation:	Continuous				
Materials Handled:					
		Inlet	Outlet 1	Outlet 2	Outlet 3
Temperature (°C)		25	25	25	25
Pressure (atm)		1	1	1	1
Component Mass Flow (kg/hr)					
Water		75,054	0	75,054	0
PHA		958	958	0	0
Lipids		479	479	0	0
De-Oiled Biomass		3,353	0	0	3,353
Design Data:					
	Height (m)		16.8		
	Radius (m)		3.4		
	Material of Construction		304 Stainless Steel		
	Design Pressure (atm)		1		
Utilities:					
Total Purchase Cost			$447,136		
Total Bare Module Cost			$2,624,460		
Comments:					

Vessel for Chloroform Addition			
Identification:	**Item**	V-400	
	No. Req	1	
Function:	Agitated vessel for the addition of chloroform to the PHA-lipid mixture		
Operation:	Continuous		
Materials Handled:			
	Inlet 1	Inlet 2	Outlet
Temperature (°C)	25	25	25
Pressure (atm)	1	1	1
Component Mass Flow (kg/hr)			
PHA	958	0	958
Lipid	479	0	479
Chloroform	0	133,363	133,363
Design Data:			
	Height (m)	6.2	
	Radius (m)	1.5	
	Material of Construction	304 Stainless Steel	
	Design Pressure (atm)	1	
Utilities:	Electricity: 1.3 kW		
Total Purchase Cost		$138,152	
Total Bare Module Cost		$810,883	
Comments: In order to ensure that the vessel is well-mixed, an agitator (propellor) is necessary. This results in an additional purchase cost of $7,178, bare module cost of $23,688.			

Vessel for Methanol Addition			
Identification:	**Item**	V-401	
	No. Req	1	
Function:	Agitated vessel for the addition of methanol to precipitate PHA		
Operation:	Continuous		
Materials Handled:			
	Inlet 1	Inlet 2	Outlet
Temperature (°C)	25	25	25
Pressure (atm)	1	1	1
Component Mass Flow (kg/hr)			
PHA	958	0	958
Lipid	479	0	479
Chloroform	133,363	0	133,363
Methanol	0	641,495	641,495
Design Data:			
	Height (m)	11.0	
	Radius (m)	2.7	
	Material of Construction	304 Stainless Steel	
	Design Pressure (atm)	1	
Utilities:	Electricity: 7.18 kW		
Total Purchase Cost		$298,608	
Total Bare Module Cost		$1,752,677	
Comments: In order to ensure that the vessel is well-mixed, an agitator (turbine) is necessary. This results in an additional purchase cost of $43,532, bare module cost of $143,657.			

Vessel for Water Addition			
Identification:	**Item**	V-402	
	No. Req	1	
Function:	Agitated vessel for the addition of water in order to create two separate phases		
Operation:	Continuous		
Materials Handled:			
	Inlet 1	Inlet 2	Outlet
Temperature (°C)	25	25	25
Pressure (atm)	1	1	1
Component Mass Flow (kg/hr)			
Lipid	479	0	479
Chloroform	132,029	0	133,363
Methanol	641,495	0	641,495
Water	0	810,992	810,992
Design Data:			
	Height (m)	13.9	
	Radius (m)	3.5	
	Material of Construction	304 Stainless Steel	
	Design Pressure (atm)	1	
Utilities:	Electricity: 14.6 kW; Process water		
Total Purchase Cost		$416,617	
Total Bare Module Cost		$2,445,332	
Comments: In order to ensure that the vessel is well-mixed, an agitator (turbine) is necessary. This results in an additional purchase cost of $65,336, bare module cost of $215,610.			

Decanter			
Identification:	**Item**	V-403	
	No. Req	1	
Function:	Agitated vessel for the addition of water in order to create two separate phases		
Operation:	Continuous		
Materials Handled:			
	Inlet	Outlet 1	Outlet 2
Temperature (°C)	25	25	25
Pressure (atm)	1	1	1
Component Mass Flow (kg/hr)			
Lipid	479	0	479
Chloroform	133,363	0	133,363
Methanol	641,495	641,495	0
Water	810,992	810,992	0
Design Data:			
	Height (m)	13.9	
	Radius (m)	3.5	
	Material of Construction	304 Stainless Steel	
	Design Pressure (atm)	1	
Utilities:			
Total Purchase Cost		$203,122	
Total Bare Module Cost		$874,105	
Comments:			

Centrifuges

Centrifuge for Algae Dewatering			
Identification:	**Item**	C-300	
	No. Req	1	
Function:	Dewatering the algae slurry to 80 wt% water, with a recycle of 99.96 wt% water		
Operation:	Continuous		
Materials Handled:			
	Inlet	Outlet 1	Outlet 2
Temperature (°C)	25	25	25
Pressure (atm)	1	1	1
Component Mass Flow (kg/hr)			
Algae	4,898	4,791	107
Water	286,958	75,054	267,796
Design Data:			
	Type	Bowl Centrifuge	
	Material of construction	304 Stainless Steel	
Utilities:	Electricity: $2,713,684		
Total Purchase Cost	$1,901,333		
Total Bare Module Cost	$5,445,796		
Comments:			

Centrifuge for PHA Removal			
Identification:	**Item**	C-400	
	No. Req	1	
Function:	Centrifuge for the removal of the precipitated PHA		
Operation:	Continuous		
Materials Handled:			
	Inlet	Outlet 1	Outlet 2
Temperature (°C)	25	25	25
Pressure (atm)	1	1	1
Component Mass Flow (kg/hr)			
PHA	958	0	958
Chloroform	1,334	1,334	0
Design Data:			
	Type	Continuous Reciprocating Pusher	
	Tons solids/hr	1.1	
	Material of Construction	304 Stainless Steel	
Utilities:	Electricity: $7,341,203		
Total Purchase Cost		$172,922	
Total Bare Module Cost		$495,283	
Comments:			

Towers

Distillation Column for Methanol and Water Separation			
Identification:	**Item**	T-400	
	No. Req	4	
Function:	Separation of methanol and water for recycle		
Operation:	Continuous		
Materials Handled:			
	Inlet	Outlet 1	Outlet 2
Temperature (°C)	25	64.7	99.5
Pressure (atm)	1	1	1
Component mass flow (kg/hr)			
Water	202,748	1,193	201,555
Methanol	160,374	159,307	1,067
Design Data:			
	Height (m)	17.5	
	Diameter (m)	4.3	
	Material of Construction	304 Stainless Steel	
	Design Pressure (atm)	1	
	Tray Type	Sieve	
Utilities:	Heat Duty: E-401 (-396,054.4 kW), E-402 (492,552.0 kW)		
Total Purchase Cost		$3,780,688	
Total Bare Module Cost		$22,190,705	
Comments: The purchasing cost for the condenser (E-401) was $928,974, with a bare module cost of $1,997,293. The purchasing cost for the reboiler (E-402) was $344,927, with a bare module cost of $741,593.			

Distillation Column for Chloroform and Lipid Separation			
Identification:	**Item**	T-401	
	No. Req	1	
Function:	Separation of chloroform (for recycle) and triolein (for byproduct isolation)		
Operation:	Continuous		
Materials Handled:			
	Inlet	Outlet 1	Outlet 2
Temperature (°C)	25	61.1	240.9
Pressure (atm)	1	1	1
Component mass flow (kg/hr)			
Chloroform	132,030	132,016	14
Triolein	479	0	479
Design Data:			
	Height (m)	10.7	
	Radius (m)	2.1	
	Material of Construction	304 Stainless Steel	
	Design Pressure (atm)	1	
	Tray Type	Sieve	
Utilities:	Heat Duty: E-403 (-16,235.8 kW), E-404 (17,630.9 kW)		
Total Purchase Cost		$406,007	
Total Bare Module Cost		$2,383,058	
Comments: The purchasing cost for the condenser (E-403) was $65,000, with a bare module cost of $139,750. The purchasing cost for the reboiler (E-404) was $248,142, with a bare module cost of $533,505.			

Heat Exchangers

Evaporator for PHA Drying			
Identification:	**Item** No. Req	E-400 1	
Function:	Evaporate the remaining chloroform solvent from the isolated PHA		
Operation:	Continuous		
Materials Handled:			
	Inlet	Outlet 1	Outlet 2
Temperature (°C)	25	60	60
Pressure (atm)	1	1	1
Component Mass Flow (kg/hr)			
PHA	958	958	0
Chloroform	1,334	0	1,334
Design Data:			
	Type	Continuous Evaporative Draft-Tube Baffled	
	Tons of Crystals/Day	25.4	
	Design Temperature (°C)	60	
Utilities:	Electricity: $50,729		
Total Purchase Cost		$245,142	
Total Bare Module Cost		$847,406	
Comments:			

Economics

Equipment Cost Summary

The bare module factors listed here were found from Seider et al, 2017 and consultation with Bruce Vrana. The majority of purchasing costs were also determined through Seider et al, 2017 by following procedures for sizing equipment and using the costing equations. Flat plate PBR installation costs were determined from an estimate by the University of Florence cited by the National Renewable Energy Laboratory (Clippinger & Davis, 2019).

A breakdown of purchase and bare module costs by equipment is shown in Table 7. Equipment prices were calculated with a cost index of CE = 800, which was given by faculty advisors.

Note that a sonicator and FTIR spectroscopy machine were also necessary, though specifications were not included. An allowance of $120,000 and $24,000 were set aside for those two pieces of equipment. These are "bare module costs" after a bare module factor of 1.2.

Table 77. Purchasing Costs and Bare Module Costs of Equipment

Unit ID	Unit Type	Equipment Description	Purchasing Cost ($)	Bare Module Factor	Bare Module Cost ($)
R-100	Reactor	Flat plate photobioreactors	$35,607,679	2.3	$81,897,662
TK-200	Storage tank	Storage tank for flue gas	$396,507	4.0	$2,237,785
TK-201	Tank	Medium preparation tank	$297,755	1.2	$502,982
P-200	Centrifugal pump	Feed pumps to photobioreactors	$88,810	3.3	$413,506
V-200	Vessel	Gravity settler for harvesting	$396,423	1.2	$665,908
P-201	Centrifugal pump	Algae recirculation pump	$660,170	3.3	$3,073,807
P-202	Centrifugal pump	Harvested algae pump	$86,120	3.3	$400,982
C-300	Centrifuge	Centrifuge for dewatering	$1,901,333	2.03	$5,445,796
P-300	Centrifugal pump	Algae recycle pump to cultivation	$86,110	3.3	$400,935
V-300	Vertical pressure vessel	Extraction vessel	$97,861	4.16	$574,399
V-301	Vertical pressure vessel	Gravity settler	$447,136	4.16	$2,624,459
V-400	Vertical pressure vessel	Vessel for chloroform addition	$138,152	4.16	$810,883
V-401	Vertical pressure vessel	Vessel for methanol addition	$298,608	4.16	$1,752,677
C-400	Centrifuge	Centrifuge for PHA isolation	$172,922	2.03	$495,283

E-400	Evaporator	Evaporator for PHA drying	$245,142	2.45	$847,406
V-402	Vertical pressure vessel	Vessel for water addition	$416,617	4.16	$2,445,332
V-403	Horizontal pressure vessel	Decanter	$203,122	3.05	$874,105
T-400	Distillation column	M/W Distillation column	$15,122,752	4.16	$88,762,821
E-401	Condenser	Condenser for T-400	$2,633,639	2.15	$7,989,172
E-402	Reboiler	Reboiler for T-400	$977,868	2.15	$2,966,373
T-401	Distillation column	C/L Distillation column	$406,007	4.16	$2,383,058
E-403	Condenser	Condenser for T-401	$46,068	2.15	$139,750
E-404	Reboiler	Reboiler for T-401	$175,870	3.17	$533,505
	Other	Sonicator	$100,000	1.2	$120,000
	Other	FTIR Spectroscopy Machine	$20,000	1.2	$24,000

Fixed-Capital Investment Summary

The fixed capital investment for the project was determined using the procedure described in Seider et al., 2017. The costs included in the total capital investment are shown in Table 8 below. In addition to the equipment and machinery costs of the plant, costs for the plant site, facilities, contractors, and land must be accounted for. The percent of each factor is included in the table. 1-yr design and 1-yr construction periods were used for this plant.

Table 88. Total Permanent Investment Breakdown for Proposed Plant

Process Machinery	\$267,494,820
Storage	\$2,237,786
Other Equipment (Sonicator, FTIR Spectrometer)	\$144,000
Total Bare Module Costs	\$269,876,605
Cost of Site Preparations ($0.05C_{TBM}$)	\$13,493,830
Cost of Service Facilities ($0.05C_{TBM}$)	\$13,493,830
Direct Permanent Investment	\$296,864,266
Cost of Contingencies & Contractor Free ($0.18C_{DPI}$)	\$53,435,568
Total Depreciable Capital	\$350,299,834
Cost of Land ($0.02C_{TDC}$)	\$7,005,997
Cost of Plant Startup ($0.10C_{TDC}$)	\$35,029,983
Total Permanent Investment	\$392,335,814
Total Permanent Investment (Adjusted for Site Factor)	\$387,694,341

After adjustment for a site factor of 0.95, the total permanent investment is \$388 million. Once total permanent investment is calculated, working capital must be evaluated in order to find the total capital investment for the plant. The working capital includes 30 days of accounts receivable, cash reserves, and accounts payable, four days of PHA inventory and two days of raw materials inventory. These calculations are shown below in Table 9.

Table 99. Working Capital Calculation for Proposed Plant

	2023	2024	2025
Accounts Receivable	$3,087,122.31	$1,543,561.15	$1,543,561.15
Cash Reserves	$411,616.31	$205,808.15	$205,808.15
Accounts Payable	$75,389.97	$37,694.98	$37,694.98
PHA Inventory	$370,586.91	$185,293.45	$185,293.45
Raw Materials	$1,130,849.51	$565,424.75	$565,424.75
Total	$2,813,865.98	$1,406,932.99	$1,406,932.99
Present Value at 15%	$2,446,839.98	$1,063,843.47	$925,081.28

By adding the present values for each year of working capital, these are combined with the total permanent investment to arrive at a total capital investment of $392,130,106.

Operating Cost

The operating costs, otherwise known as the costs of manufacture, were determined for the proposed plant. Despite the large investment costs, this plant has small production rates, with annual production capacities of 8,366 US tons of PHAs, 29,283 US tons of de-oiled biomass, and 4,183 US tons of lipid (triolein).

There is a fair amount of recycle of chloroform and methanol, but each raw material is still necessary in large quantities. The raw materials required for the plant are shown in Table 10 below.

Table 10. Summary of Raw Material Costs for Proposed Plant

Feedstock	Annual Costs ($/yr)	Unit Cost (per kg of PHA)
Chloroform	$9,975,955	$1.31
Methanol	$14,902,735	$1.96
Total Feedstock Costs	**$24,878,689**	**$3.28**

The utilities for the plant were one of the largest factors in the operating cost, displayed in Table 11. Costing for these utilities were pulled from Seider et. al., 2017 (Chapter 17). Breakdowns for the utilities by equipment can be seen in Table 4.

Table 11. Summary of Utility Costs for Proposed Plant

Utility	Annual Costs ($/yr)	Unit Cost (per kg of PHA)
Electricity	$13,572,367	$1.79
Cooling Water	$4,429,029	$0.58
High Pressure Steam	$14,904,952	$1.96
Process Water	$11,119	$0.01
Total Utility Costs	**$32,917,468**	**$4.34**

The plant's variable costs are made up of raw materials and utilities, as well as the consideration of general expenses. These variable costs are summarized in Table 12.

Table 12. Annual Variable Costs of Proposed Plant

General Expenses	$4,732,921
Selling/Transfer Expenses	$1,229,330
Direct Research	$1,966,928
Allocated Research	$204,888
Administrative Expense	$819,553
Management Incentive Compensation	$512,221
Raw Materials	$24,878,689
Byproducts	($26,939,022)
Utilities	$32,917,468
Total Variable Costs	**$35,590,055**

In addition to the variable costs, there are a number of fixed costs for the operation of the plant, which comprise operations, maintenance, and insurance. These fixed operating costs, summarized in Table 13 below, were similarly calculated with approximations in Seider et. al., 2009.

Table 13. Summary of Fixed Operating Costs for Proposed Plant

Total Operations Costs	$2,475,000
Direct Wages and Benefits	$1,500,000
Direct Salaries and Benefits	$225,000
Operations Supplies and Services	$90,000.00

Technical Assistance to Manufacturing	$360,000
Control Laboratory	$300,000
Total Maintenance Costs	$982,100
Wages and Benefits	$427,000
Salaries and Benefits	$106,750
Material and Services	$427,000
Maintenance Overhead	$21,350
Total Operating Overhead Costs	$439,356
General Plant Overhead	$136,817
Mechanical Department Services	$46,248
Employee Relations Department	$113,693
Business Services	$142,598
Property Taxes and Insurance	$180,000
Insurance	$180,000
Total Fixed Costs	**$4,076,456**

Profitability Analysis

A profitability analysis was performed as a business case for the proposed plant. The goal of this project was to obtain a 15% IRR by selling byproducts alongside the primary product. The profitability of the plant is largely dependent on the selling prices of PHA and the byproducts (de-oiled microalgal biomass and triolein). In the costing scenario discussed here, PHA, DMB, and triolein are assumed to be sold at a market unit price. Table 14 summarizes the revenue streams of the process.

Table 14. Summary of Revenue Steams (PHA and Byproducts)

Byproducts/Products	Unit Price (per kg)	Ratio (per kg of PHA)	Annual Sales
De-Oiled Biomass[a]	\$1.50	0.5	\$21.25 M
Triolein[b]	\$0.80	3.5	\$5.69 M
PHA[c]	\$5.40	1	\$40.98 M

[a] Yadav et. al., 2021, [b] Karamerou et. al., 2021, [c] Khatami et. al., 2021

The capital costs of the plant were also a key factor. This included equipment costs and capital expenditures, among other costs. The lifetime of the plant was set at 20 years, with two years prior for design and construction. The tax rate (24%) and depreciation value (5-year MACRS) were also factors in the plant's profitability.

General Information							
		Process Title:	**Production of PHA from Microalgae**				
		Product:	**PHA**				
		Plant Site Location:	**Coolidge, Arizona**				
		Site Factor:	**0.95**				
		Operating Hours per Year:	**7920**				
		Operating Days Per Year:	**330**				
		Operating Factor:	**0.9041**				
Product Information							
This Process will Yield							
		958	kg of PHA per hour				
		22,992	kg of PHA per day				
		7,587,360	kg of PHA per year				
	Price	**$5.40**	**/kg**				
Chronology							
		Distribution of		**Production**	**Depreciation**		**Product Pri**
Year	**Action**	**Permanent Investment**		**Capacity**	5 year MACRS		
2023	Design			0.0%			
2024	Construction	100%		0.0%			
2025	Production	0%		45.0%	20.00%		$5.40
2026	Production	0%		67.5%	32.00%		$5.40
2027	Production	0%		90.0%	19.20%		$5.40
2028	Production			90.0%	11.52%		$5.40
2029	Production			90.0%	11.52%		$5.40
2030	Production			90.0%	5.76%		$5.40
2031	Production			90.0%			$5.40
2032	Production			90.0%			$5.40
2033	Production			90.0%			$5.40
2034	Production			90.0%			$5.40
2035	Production			90.0%			$5.40
2036	Production			90.0%			$5.40
2037	Production			90.0%			$5.40
2038	Production			90.0%			$5.40
2039	Production			90.0%			$5.40

Figure 16. General Input Specifications for Plant Operations

The profitability analysis also considered operating costs from raw materials, utilities, and the sale of byproducts. This cost information is summarized in Table 15.

Table 15. Costing for Raw Materials and Utilities

	Unit	Ratio (per kg of PHA)	Cost (per unit)
Raw Materials			
ADC	kg	1,008	$0
Flue Gas	kg	250	$0
Chloroform	kg	1.39	$0.94
Methanol	kg	6.84	$0.44
Utilities			
Cooling Water[a]	gal	3062	$1E-4
High-Pressure Steam[a]	lb	972	$8E-3
Process Water[a]	gal	513	$8E-4
Electricity[a]	kWh	23.6	$0.07

[a] Seider et. al., 2017

Figure 17 shows the cash flow summary of the plant modeled in this design study. Note that a 15% discount rate was used to calculate the cumulative net present value (NPV). As expected, the significant photobioreactor cost (approximately half of the total bare modulus cost) makes it unlikely for the initial capital cost to be recouped in a reasonable timeframe. However, in addition to this upfront cost, the distillation columns at the end of the separation train not only make up a quarter of the total bare modulus cost, but also drive half of the total variable operating costs of the overall process:

Because of the large volume of solvent necessary to precipitate out the PHA (both methanol and chloroform), the utility cost for the reboiler and condenser of both distillation columns are excessive and cannot be mitigated without a reduction in the quantity of the feed. In fact, the triolein byproduct stream is still only 97.2% pure, which is unacceptable given the impurity is chloroform. Because of the high boiling point of this triglyceride (and the potential of degradation at high temperatures), the reboiler temperature had to be limited which correspondingly capped the purity of the triolein bottoms product. Although outside of the scope of this project, this byproduct would need to be treated further in order to be in acceptable condition for purchase. Alternatively, the choice of distillation itself as the method of separation can be critiqued, with newer and more nuanced methods gaining popularity as a way of reducing energy costs: such methods include distillation paired with mechanical compression and membrane separation, which has been shown to cut the energy costs of a methanol/water separation in half (Huang et. al., 2010).

Year	Percent Design Capacity	Product Price	Sales	Capital Costs	Working Capital	Var Costs	Fixed Costs	Depreciation	Taxible Income	Taxes	Net Earnings	Cash Flow	Cumulative Net Present Value
2023			-	-	-	-	-	-	0	0	0	0	0
2024			-	(392,130,106)	(2,813,866)	-	-	-	0	0	0	(394,943,972)	(394,943,972)
2025	45%	$5.40	30,562,511	-	(1,406,933)	(16,015,525)	(4,076,456)	(78,426,021.12)	(67,955,491)	15,629,763	(52,325,728)	24,693,360	(373,471,485)
2026	68%	$5.40	45,843,766	-	(1,406,933)	(24,023,287)	(4,076,456)	(125,481,633.79)	(107,737,611)	24,779,650	(82,957,960)	41,116,741	(342,381,322)
2027	90%	$5.40	61,125,022	-	-	(32,031,049)	(4,076,456)	(75,288,980.28)	(50,271,464)	11,562,437	(38,709,027)	36,579,953	(318,329,409)
2028	90%	$5.40	61,125,022	-	-	(32,031,049)	(4,076,456)	(45,173,388.17)	(20,155,872)	4,635,851	(15,520,021)	29,653,367	(301,375,000)
2029	90%	$5.40	61,125,022	-	-	(32,031,049)	(4,076,456)	(45,173,388.17)	(20,155,872)	4,635,851	(15,520,021)	29,653,367	(286,632,036)
2030	90%	$5.40	61,125,022	-	-	(32,031,049)	(4,076,456)	(22,586,694.08)	2,430,822	(559,089)	1,871,733	24,458,427	(276,057,983)
2031	90%	$5.40	61,125,022	-	-	(32,031,049)	(4,076,456)	-	25,017,516	(5,754,029)	19,263,487	19,263,487	(268,816,124)
2032	90%	$5.40	61,125,022	-	-	(32,031,049)	(4,076,456)	-	25,017,516	(5,754,029)	19,263,487	19,263,487	(262,518,856)
2033	90%	$5.40	61,125,022	-	-	(32,031,049)	(4,076,456)	-	25,017,516	(5,754,029)	19,263,487	19,263,487	(257,042,971)
2034	90%	$5.40	61,125,022	-	-	(32,031,049)	(4,076,456)	-	25,017,516	(5,754,029)	19,263,487	19,263,487	(252,281,331)
2035	90%	$5.40	61,125,022	-	-	(32,031,049)	(4,076,456)	-	25,017,516	(5,754,029)	19,263,487	19,263,487	(248,140,775)
2036	90%	$5.40	61,125,022	-	-	(32,031,049)	(4,076,456)	-	25,017,516	(5,754,029)	19,263,487	19,263,487	(244,540,292)
2037	90%	$5.40	61,125,022	-	-	(32,031,049)	(4,076,456)	-	25,017,516	(5,754,029)	19,263,487	19,263,487	(241,409,436)
2038	90%	$5.40	61,125,022	-	-	(32,031,049)	(4,076,456)	-	25,017,516	(5,754,029)	19,263,487	19,263,487	(238,686,954)
2039	90%	$5.40	61,125,022	-	-	(32,031,049)	(4,076,456)	-	25,017,516	(5,754,029)	19,263,487	19,263,487	(236,319,577)
2040	90%	$5.40	61,125,022	-	-	(32,031,049)	(4,076,456)	-	25,017,516	(5,754,029)	19,263,487	19,263,487	(234,260,989)
2041	90%	$5.40	61,125,022	-	-	(32,031,049)	(4,076,456)	-	25,017,516	(5,754,029)	19,263,487	19,263,487	(232,470,912)
2042	90%	$5.40	61,125,022	-	-	(32,031,049)	(4,076,456)	-	25,017,516	(5,754,029)	19,263,487	19,263,487	(230,914,324)
2043	90%	$5.40	61,125,022	-	-	(32,031,049)	(4,076,456)	-	25,017,516	(5,754,029)	19,263,487	19,263,487	(229,560,769)
2044	90%	$5.40	61,125,022	-	-	(32,031,049)	(4,076,456)	-	25,017,516	(5,754,029)	19,263,487	19,263,487	(228,383,764)

Figure 17. Cash Flow Summary of Example Case for Plant

Given that the variable costs for this process are as large as presented, one can look towards the total capital invement cost as a potential avenue for approaching the IRR goal of 15%. A sensitivity analysis was performed where the capital investment in this study ($392 M) was arbitrarily cut down to investigate the potential profitability of this process. Figure 18 shows that, at 42% of the original capital investment (i.e., $164 M), the desired IRR of 15% is achieved. This result is justified by the relatively high unit margin of $3.01 per kg of PHA, given that the production rate is nearly 7.6 M kg/hr. This balance between production rate and unit margin also brings up the potential associated with the initial productivity of the cultivation process.

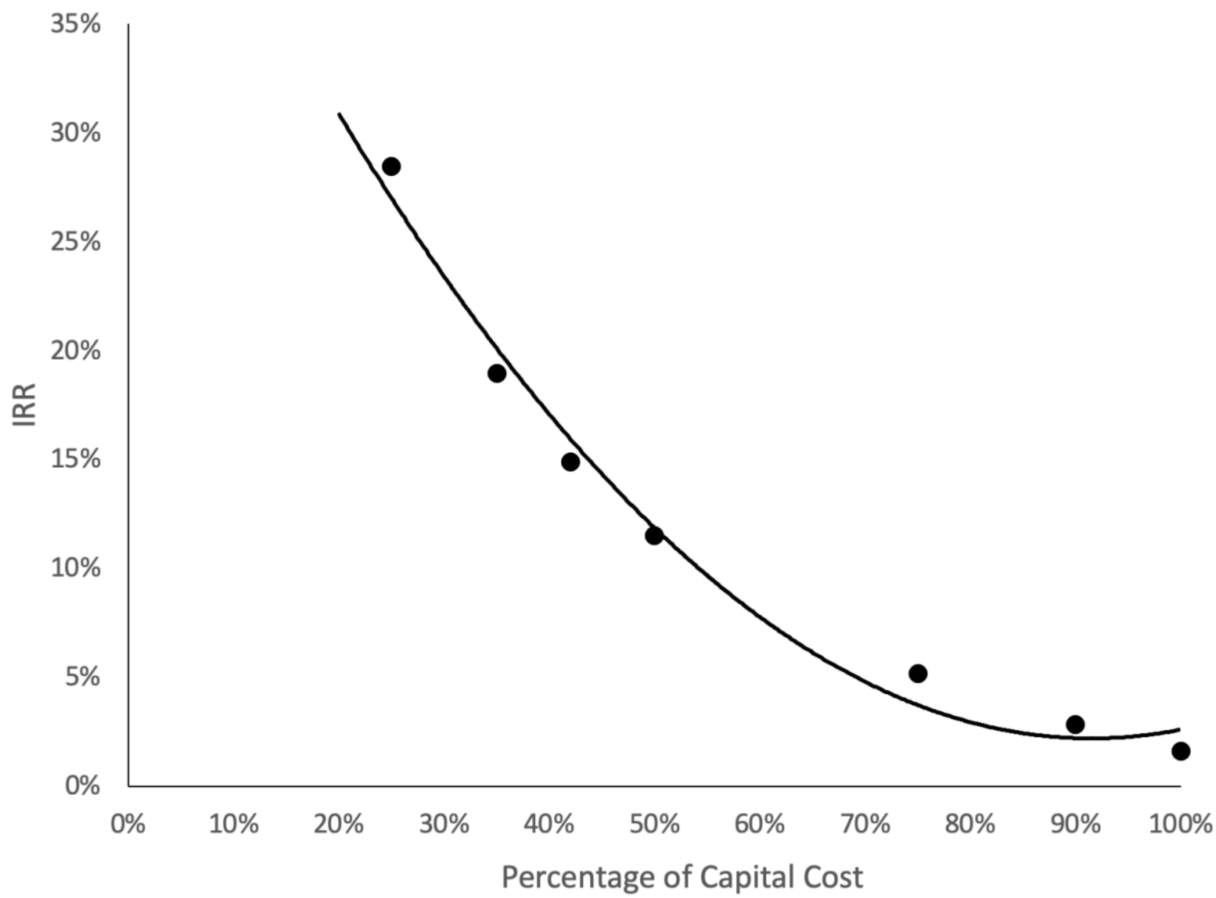


Figure 18. Sensitivity analysis for the IRR in response to a reduction in the total capital cost

Table 16 is a side-by-side comparison of two biomass productivities and their associated economics. It is clear that the 0.5 g/L/day case is significantly less economically favorable, which raises the question of whether a higher productivity than is currently achievable would make this algae-based process economical.

Table 16. Comparison of Economics of Two Biomass Productivity Cases

Biomass Productivity	**0.5 g/L/day**	**1.81 g/L/day**
Production		
Annual PHA Production (kg)	2,126,032	7,588,457
Economics (Costs)		
Annual Cost of Raw Materials	$9,186,946	$24,878,689
Annual Cost of Utilities	$25,537,305	$32,917,468
Total Annual Variable Costs	$28,502,842	$35,590,055
Unit Cost (per kg of PHA)	$13.41	$4.70
Total Bare Modulus Cost	$216,034,447	$269,876,605
Total Capital Investment (TCI)	$311,861,791	$392,130,106
Economics (Revenues)		
Annual PHA Revenue	$11,480,575	$40,977,668
Annual Byproduct Revenue	$7,547,415	$26,939,023
Unit Margins (per kg of PHA)	($5.31)	$3.01

Acknowledging that the bulk of the costs in this process were incurred in the cultivation portion, the economics were considered without these costs in order to provide an estimate that may be more similar to the cost of a production process using bacteria instead of algae. This hypothetical gave a capital cost of $175.6 M instead of $392.1 M, which is a 55% reduction. This is even without considerations of the corresponding decrease in additional fixed costs and operating costs. This displays the potential magnitude of our disadvantage compared to current competitors in the market — Danimer Scientific and Mango Materials, as discussed above — who are using bacteria instead of algae for their processes.

Additional Considerations

Safety and Health Concerns

Stacks may be necessary for gas purge in order to maintain a safe concentration of oxygen at breathing level for the sake of employee safety, as well as the safety of the public in the surrounding area.

Despite attempts to find solvents which would be less problematic, chloroform and methanol was the only combination of solvents that has been adequately researched for our purposes. Chloroform is very bad for the environment. Caution must be taken with the triolein product, even though the amount of chloroform contained in it can be considered negligible. For this reason, it will not be sold to industries which make products that involve ingestion or skin contact. Methanol is toxic, so it is important consider the purge stream to determine how we can safely dispose of it or sell it in its diluted form. It can be fatal to animals and detrimental to plants if it enters a public water source. If purged, we would need to ensure that it is well-treated at its destination.

Environmental Factors

The issues discussed above are also considered as environmental factors. The gas purge will be a significant source of emissions, but since it was already diverted from another plant, it was bound for the atmosphere regardless.

Methanol and chloroform are not environmentally sound. It will be important to avoid any sort of chloroform emissions from the plant.

Conclusions and Recommendations

As the climate crisis and the plastic pollution problem become increasingly dire, biodegradable polymers, specifically PHAs, have become an attractive alternative to traditional petroleum-based polymers. This project presents a proposed process for the production of PHA from the green microalgae species *Scenedesmus* on an industrial scale.

This process employs the use of flat plate photobioreactors for algae cultivation, gravity settling and centrifugation for harvesting and dewatering, microbubble extraction for cell lysis, and a separation train for the purification of PHA from lipids. The annual production capacity is 8,366 US tons of PHAs, 29,283 US tons of de-oiled biomass, and 4,183 US tons of triolein.

The primary goal of this report was to achieve a 15% internal rate of return (IRR). However, with a total capital investment of $392.1 million and an annual profit margin of $19.3 million, this project is not economical. The internal rate of return was 1.6% with reasonable selling prices of the product. We would not recommend moving forward with this design unless significant changes are made, including but not limited to changes to the major contributors to capital cost (photobioreactors, distillation columns) and utility costs (use of high-pressure steam).

After exploring the use of microalgae in the production of PHA, we have determined that a more economical way to produce PHA is with bacteria, due to the dramatic reduction in land and equipment use (most notably the photobioreactors). This scenario is partially simulated in the profitability analysis section when determining the total capital cost in the absence of cultivation costs ($175.6 M instead of $392.1 M). However, within the realm of PHA production from algae, future recommendations for research include further exploration into alternative cultivation methods (e.g., open raceway ponds) and alternative lipid-PHA separation techniques that could be optimized for the throughput of this industrial-scale process. Additionally, as the market shifts towards sustainable products, the increased selling prices of the products would make the project more profitable without having to change the process itself.

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Appendix

Problem Statement

8. Polyhydroxyalkanoate (PHA) – A Biodegradable Polymer
(Recommended by W. D. Seider, UPenn and Geetanjali Yadav, NREL)

Traditionally, plastics are derived from petroleum feedstocks. About 6% of the world fossil fuel consumption is used to make polymers (equivalent to the global aviation sector)[1] and it is projected to increase to 20% global fossil consumption by 2050. In 2016, the US generated the most plastic waste globally (about 42 million metric tons)[2]. Polyhydroxyalkanoates (PHAs), biodegradable biopolymers from blue-green algae (cyanobacteria) cells and bacteria, are gaining popularity as substitutes for conventional fossil-derived polymers. In recent years, several hundred products have appeared for an array of applications, including extrusion coatings, extrusion lamination materials, film resins, and injection molding resins. Over the past decade, worldwide companies (e.g., Danimer and Mango Materials in the U.S.) have positioned themselves to provide an important alternative to upcycling of conventional plastic products.

Production costs for PHAs are still very high, largely due to the cost of carbon feedstocks for the bacteria that produce the polymers, and the cost of extracting the polymers after production. The goal of this design project is to synthesize a process to produce PHAs from green microalgal biomass. Researchers (Garcia et al., 2021)[3] have reported the production of PHAs from *Scenedesmus* sp. for the first time after careful evaluation of critical nutritional parameters that result in increased PHA accumulation within the algae cells[3]. Although PHA accumulation occurs naturally in photosynthetic organisms, such as microalgae, their yield can be improved in response to nutrient deficiency conditions in the presence of a carbon source.

As seen in Figure 1, the synthesis of PHA in photosynthetic microorganisms starts with the consumption of acetyl-CoA, grown in a glycolysis fermentation of glucose. Two acetyl-CoA molecules are joined together to form one acetoacetyl-CoA molecule in a β-ketothiolase (PhaA) catalyzed condensation reaction. This molecule is then reduced to R-3-hydroxybutyryl-CoA by nicotinamide adenine dinucleotide phosphate (NADPH)-dependent acetoacetyl-CoA reductase (PhaB). Finally, PHB synthase (PhaC) catalyzes the binding of R-3-hydroxybutyryl to an existing polyhydroxybutyrate (PHB) molecule through an ester bond, releasing HSCoA. The chemical composition of the resulting PHA polymers can be manipulated by varying the substrates fed to the *Scenedesmus* sp. algae. Since the synthesis of PHA is regulated at the enzymatic level, the intracellular concentration of acetyl-CoA and free CoA plays a central role in the synthesis of the polymer. The enzymatic activity and the availability of the PHA precursors are dependent on the presence of different compounds (such as glucose, glycerol, and the like) in the growth medium[3].

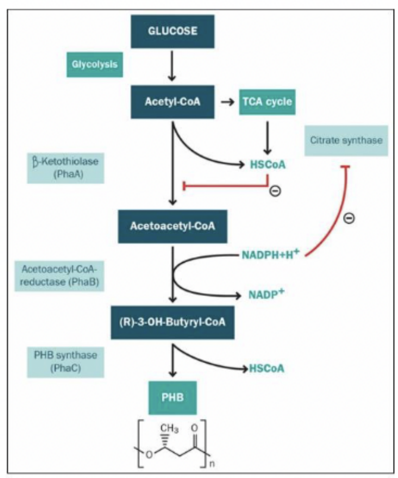

Figure 1. PHA/PHB synthesis pathway from acetyl-CoA in microalgae.

The process to be designed should use their laboratory data to scale-up an industrial process that utilizes closed airlift photobioreactors, light and nutrients (especially glucose) for the cultivation of algae biomass and simultaneous accumulation of PHA within the cells. *Scenedesmus* sp. do not require supplementation with large amounts of exogenous carbon to produce PHA, an economical advantage over the use of higher accumulating bacteria. Also, its tolerance to salinity stress makes its cultivation possible using seawater/wastewater, instead of freshwater. Further, it also produces other valuable metabolites such as lipids and carbohydrates – macromolecules of interest for the production of biofuel and bioethanol, thereby improving the spectrum of utilizing co-product credits.

Next, the microalgal biomass must be harvested using one of the several dewatering techniques such as dissolved air flotation, froth-flotation, etc. The dewatered biomass should undergo downstream processing to disrupt the cells for recovering a mixture of metabolites including PHAs, lipids and carbohydrates. Finally, this mixture should be separated from the residual slurry employing appropriate techniques and/or solvents to recover high purity PHAs ready to be packaged after drying[4]. The remaining culture medium should be recycled to the cultivation step.

The objective will be to demonstrate PHA production ($/kg of PHA) through microalgae growth achieving an economically favorable internal rate of return (IRR) of the PHA plant, with a minimum of 15% IRR. The design project must incorporate an adequate consideration of each one of the processing stages, their yields, and the market value of the obtained copolymers that have desired polymer properties (e.g., average molecular weight, glass transition and melting temperatures[5]) during economic evaluation.

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Acronyms

Abbreviation	Word/Phrase
ADC	Anaerobic Digestion Centrate
DMB	Dried Microalgal Biomass
DO	Dissolved Oxygen
IRR	Investors Rate of Return
NPV	Net Present Value
OD	Optical Density
PBR	Photobioreactor
PHA	Polyhydroxyalkanoate
PLA	Polylactic Acid
ROI	Return on Investment

Design Calculations

Cultivation

Land Area	
(hectares)	100
(acres)	247.1
(m^2)	1000000
One Field (ha)	10
(m^2)	100000
Length (m)	400
Width (m)	250
Number of reactors (rows)	228
Number of units per reactor (row)	156
Volume of each row (m^3)	29.25
Total volume (m^3)	6669
Productivity	
Volumetric (g/L/day)	1.81
Mass flow rate (kg/hr)	4897.853685

R-100 – Flat Plate Photobioreactors

To determine the sizing, the land area was first considered. After determining the optimal width/length of the cultivation fields, it was found that given the spacing of 1 meter between reactors and a reactor thickness of 0.05 m, 228 rows could be placed in each field. Given the length of each reactor unit (2.5 m), 156 units could be placed in each row, leaving 10 meters on the end for harvesting. With the specs of the reactor units, (1.5 m x 2.5 m x 0.05 m), the total volume of each row (each reactor) was found to be 29.25 m^3. This results in a total cultivation volume of 6669 m^3 in each field.

With a volumetric productivity of 1.81 g/L/day (Clippinger & Davis, 2019), a mass flow rate was determined, with a dimensional analysis as follows: (1.81 g/L day)(6669 m^3/field)(10 fields)(1 kg/1000 g)(1000 L/m^3)(1 day/24 hr)*(vol fraction) = 4898 kg algae/hr.

The above referenced volume fraction is the total filled volume of each photobioreactor (R-100) — the land is graded to allow for overflow.

Grading at 1% = 0.9°

Tan(0.9°) = x / 2.5

x = 0.039273

Change in height = x / 1.5 = 0.0262

Each unit is 97.4% full

Installation costs were found in an NREL paper (Clippinger & Davis, 2019), so an F_{BM} value of 1 was assigned because purchasing costs are unknown. Subtracted portion of costing that accounted for inoculum system because that was accounted for already. See Table 4 on p.18 of NREL paper. This was done on a cost per acre basis. Attention was paid to the spacing of the PBRs due to the nature of this basis, so the cost estimate was halved since our plant was designed with 1.0 m spacing instead of 0.5 m spacing as discussed in the NREL paper, which would result in approximately half the reactors and corresponding costs.

Pumps were costed using the Equipment Costing Excel spreadsheet provided by Bruce Vrana, and using the heuristic discussed in the body of the report to determine the heads of each pump.

Dewatering

The centrifuge for dewatering **(C-300)** was sized by determining the inlet flow rate (capacity). This was done after diverting a bypass stream. The inlet flow rate was 286,958 kg/hr. This was costed using an NREL paper (Davis, et al., 2016). The centrifuge discussed in the paper had a capacity of 154,000 kg/hr at $747,500. This was scaled up using a scaling factor of 0.7.

Extraction

See supplemental materials in Yadav, et al. (2021) for the procedure followed. Vessel thicknesses were determined using the Equipment Costing Excel spreadsheet provided by Bruce Vrana.

Variable	Value	Notes/Comments
α_algae	0.061	
ρ_algae (kg/m^3)	65	
ρ_water (kg/m^3)	997.77	Different than in Yadav et al (2021) based on T and P of vessel
ρ_slurry (kg/m^3)	940.87103	
d_microbubble (m)	5.00E-05	
f_bubble generation (/s)	20000	
V_microbubble (m^3)	6.54E-14	
v_microbubble (m^3/s)	1.31E-09	
v_feed (m^3/s)	0.02	
Residence time (s)	600	Same residence time for both vessels
V_holdup (m^3)	14.14378779	
R_inner vessel (m)	1.216630268	
H_inner vessel (m)	6.083151338	Used aspect ratio (L/D) = 2.5
V_inner vessel (m^3)	14.14378779	Assumed same as holdup volume for overflow
R_GS (m)	3.358	Used Desmos: pi*(R^2 – R_E^2)*2.5*r = 2*V_holdup
H_GS (m)	16.79	Used aspect ratio (L/D) = 2.5

V_GS (m^3)	42.43136336	

V-300 - Vertical Pressure Vessel for Extraction

Variable	Value
ts (in)	0.375
ρ_ss (lb/in3)	0.286
W (lb)	10259.50064
F_M	1.7
C_V	48263.6075
C_PL	15813.73588
C_P	97861.86863

V-301 - Vertical Pressure Vessel for Gravity Settling

Variable	Value
ts (in)	0.5
ρ_ss (lb/in3)	0.286
W (lb)	99289.6143
F_M	1.7
C_V	215394.9498
C_PL	66409.42243
C_P	432580.8371

The outflow values of PHA, lipid, and DMB assumed a 20%, 10%, 70% breakdown by weight, respectively. This was determined by extrapolating the data found in Garcia, et al. (2021).

Separation

Bagley Solubility Information

	Cyclohexanone	Chloroform	PH3B	Cyclohexane
D	17.8	17.8	15.859	16.8
P	6.3	3.1	6.699	0
H	5.1	5.7	8.783	0.2
V	18.9	18.1	17.2	16.8

Solubility of PHA and Lipid in Chloroform

	Flow rate (kg/hr)	Solubility (g/L)	Source
PHA	958.1385183	11.23	https://www.observatorioplastico.com/ficheros/articulos/103093419S-4064.pdf
Lipid	479.0692591	0.1	https://www.sigmaaldrich.com/deepweb/assets/sigmaaldrich/product/documents/442/472/t7140pis.pdf

Flow Rates for Vessel Inputs

Variable	**Value**
$CHCl_3$ for PHA (L/hr)	85320
$CHCl_3$ for lipid (L/hr)	4790.692591
Total $CHCl_3$ (L/hr)	90110
Total $CHCl_3$ (gal/hr)	23804.6
Total methane (L/hr)	810992.1607
Total methane (gal/hr)	214241.4635
Total water (L/hr)	810992.1607
Total water (gal/hr)	214241.4635

V-400 – Vertical Pressure Vessel for Chloroform Addition

Variable	**Value**
Feed inflow (m^3/hr)	138.7836768
Residence time (hr)	0.1666666667
V_holdup (m^3)	23.1306128

V (2*V_holdup)	46.2612256
Radius (m)	1.544077484
Height (m)	6.176309937
Aspect ratio (L/D)	2
ts (in)	0.5
ρ_ss (lb/in^3)	0.286
W (lb)	18698.87913
F_M (304 SS)	1.7
C_V	70050.86159
C_PL	19065.85546
C_P	138152.3202

V-401 – Vertical Pressure Vessel for Methanol Addition

Variable	Value
Feed inflow (m^3/hr)	781.7122066
Residence time (hr)	0.1666666667
V_holdup (m^3)	130.2853678
V (2*V_holdup)	260.5707355
Radius (m)	2.747294763
Height (m)	10.98917905
Aspect ratio (L/D)	2
ts (in)	0.5
ρ_ss (lb/in^3)	0.286
W (lb)	59089.2921
F_M (304 SS)	1.7
C_V	149843.5897
C_PL	43874.06754
C_P	298608.17

C-400 - Continuous Reciprocating Pusher Centrifuge

Variable	Value

S (tons solids/hr)	1.056382049
C_P	172922.1463

E-400 - Continuous Evaporative Draft-Tube Baffled

Variable	Value
W (ton/day)	25.35316917
Cp	245142.5953

V-402 – Vertical Pressure Vessel for Water Addition

Variable	Value
Feed inflow (m^3/hr)	1593.750411
Residence time (hr)	0.1666666667
V_holdup (m^3)	265.6250685
V (2*V_holdup)	531.250137
Radius (m)	3.483611619
Height (m)	13.93444647
Aspect ratio (L/D)	2
ts (in)	0.5
ρ_ss (lb/in^3)	0.286
W (lb)	94961.192
F_M (304 SS)	1.7
C_V	208684.2104
C_PL	61854.49433
C_P	416617.652

V-403 – Horizontal Pressure Vessel (Decanter)

Variable	Value
Feed inflow (m^3/hr)	1593.750411
Residence time (hr)	0.1666666667
V_holdup (m^3)	265.6250685

V (2*V_holdup)	531.250137
Radius (m)	3.483611619
Height (m)	13.93444647
Aspect ratio (L/D)	2
ts (in)	0.5
ρ_ss (lb/in^3)	0.286
W (lb)	94961.192
F_M (304 SS)	1.7
C_V	116906.5136
C_PL	4380.965289
C_P	203122.0383

T-400 - Methanol-Water Distillation Column

Variable	Value
Pressure (atm)	1
Temp (C)	25
No of Stages	30
Tray Spacing (ft)	1.5
Diameter (m)	8.61
Radius (m)	4.305
Height (m)	17.52514477
ts (in)	0.5
r _ss (lb/in3)	0.286
W (lb)	146583.0466
F_M	1.7
C_V	342622.5815
C_PL	72785.15651
C_P	655243.5451
N_T	29
F_NT (>20 trays)	1
F_TT (sieve)	1
F_TM (stainless steel)	3.499990957

C_BT	30792.63626
C_T	3125444.505
C_P total	3780688.05

T-401 - Methanol-Water Distillation Column

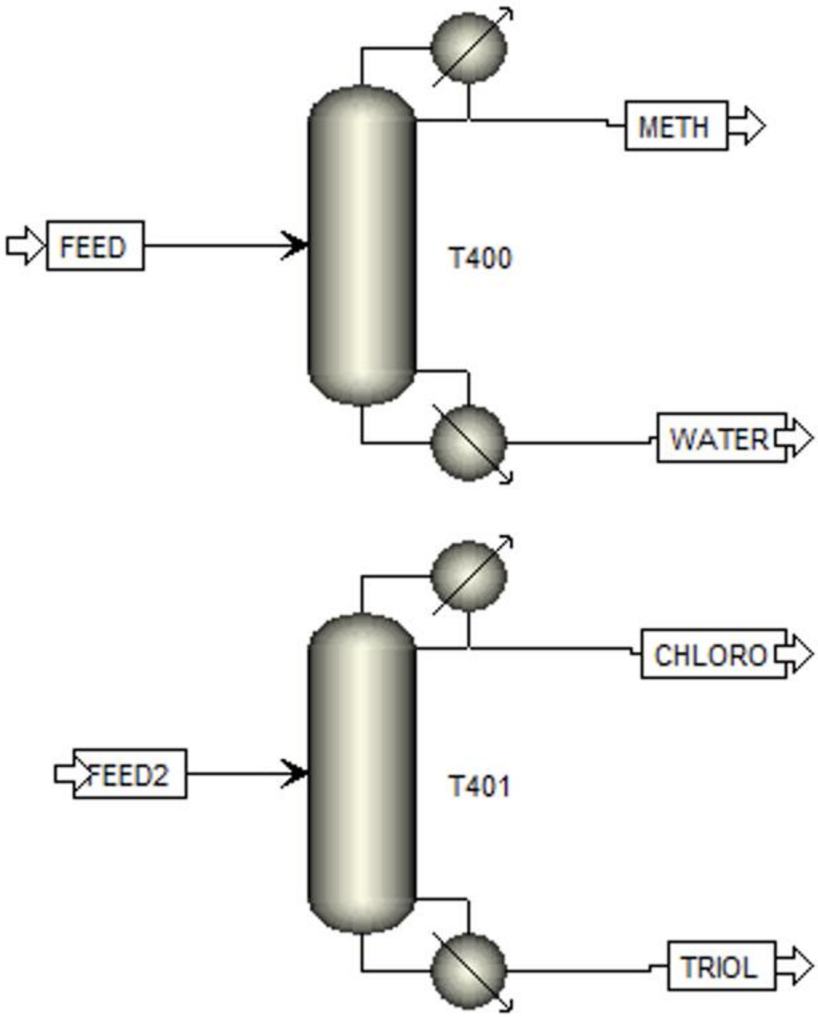
Variable	Value
Pressure (atm)	1
Temp (C)	25
No of Stages	15
Tray Spacing (ft)	1.5
Diameter (m)	4.22
Radius (m)	2.11
Height (m)	10.66747943
ts (in)	0.4375
r _ss (lb/in3)	0.286
W (lb)	36258.91763
F_M	1.7
C_V	118437.242
C_PL	31126.62979
C_P	232469.9411
N_T	14
F_NT	1.275077233
F_TT	1
F_TM	2.668903814
C_BT	3642.475529
C_T	173537.8019
C_P total	406007.743

For the reboiler and condenser of both distillation columns, the heat duty was generated by ASPEN. From these heat duties, approximate overall heat transfer coefficients were determined from Chapter 12 in Seider et. al., 2017. Assuming that a simple, countercurrent shell-and-tube heat exchanger is used with either cooling water (at 10˚C) and high-pressure steam (at 250˚C), the heat transfer area was calculated. As was specified in ASPEN, the reboilers are kettle vaporizers while the condensers are modeled as floating head, and using the equations for the base cost, C_B, and the pressure factor, F_P, in Chapter 16 of Seider et. al., 2017, the f.o.b. purchase cost was determined as shown in Table 7.

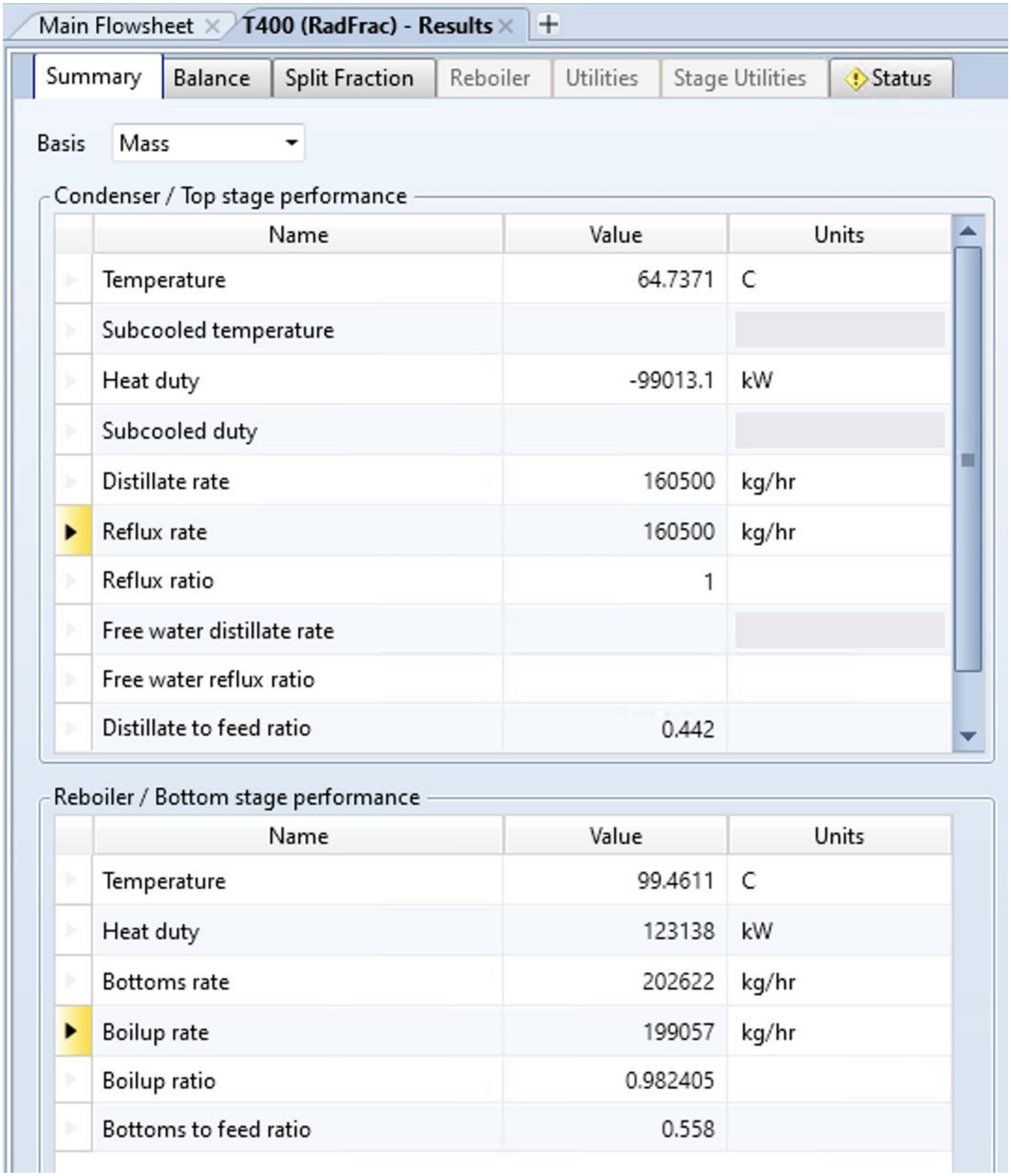
ASPEN Flowsheets and Summary Reports

Two distillation columns were designed in ASPEN Plus: one for the separation of methanol and water and one for the separation of chloroform and triolein. The methanol-water inlet stream from the decanter was split into four to have distillation columns operating in parallel in order to accommodate the large volume. Both columns were designed at atmospheric pressure, with the feed streams coming in at 25˚C. For the methanol-water distillation column, design specs were aimed at reaching a 0.99 purity in both outlet streams by varying the molar reflux ratio and distillate-to-feed ratio (by mass). After the distillate-to-feed ratio converged to 0.442, the molar reflux ratio was manually altered to reduce the diameter of the column while maintaining acceptable purities for both streams (converging to a molar reflux ratio of 1).

For the triolein-chloroform distillation column, a similar design spec was conducted by varying the molar reflux ratio and distillate-to-feed ratio (by mass) to achieve a 0.99 chloroform recovery in the distillate and a 0.99 purity of triolein in the bottoms. This specification dried out the column but still resulted in a complete pure chloroform stream (mass fraction of 1); because of this, the bottoms-to-feed ratio was manually altered until there was enough chloroform to reduce the bottoms temperature below 250˚C (i.e., the highest temperature that the high-pressure steam used in this study can heat). The molar reflux ratio converged to 0.8, while the mass distillate-to-feed ratio was determined to be 0.99628.



Supplementary Figure 1. ASPEN Process Flowsheet for Distillation Columns T-400 and T-401



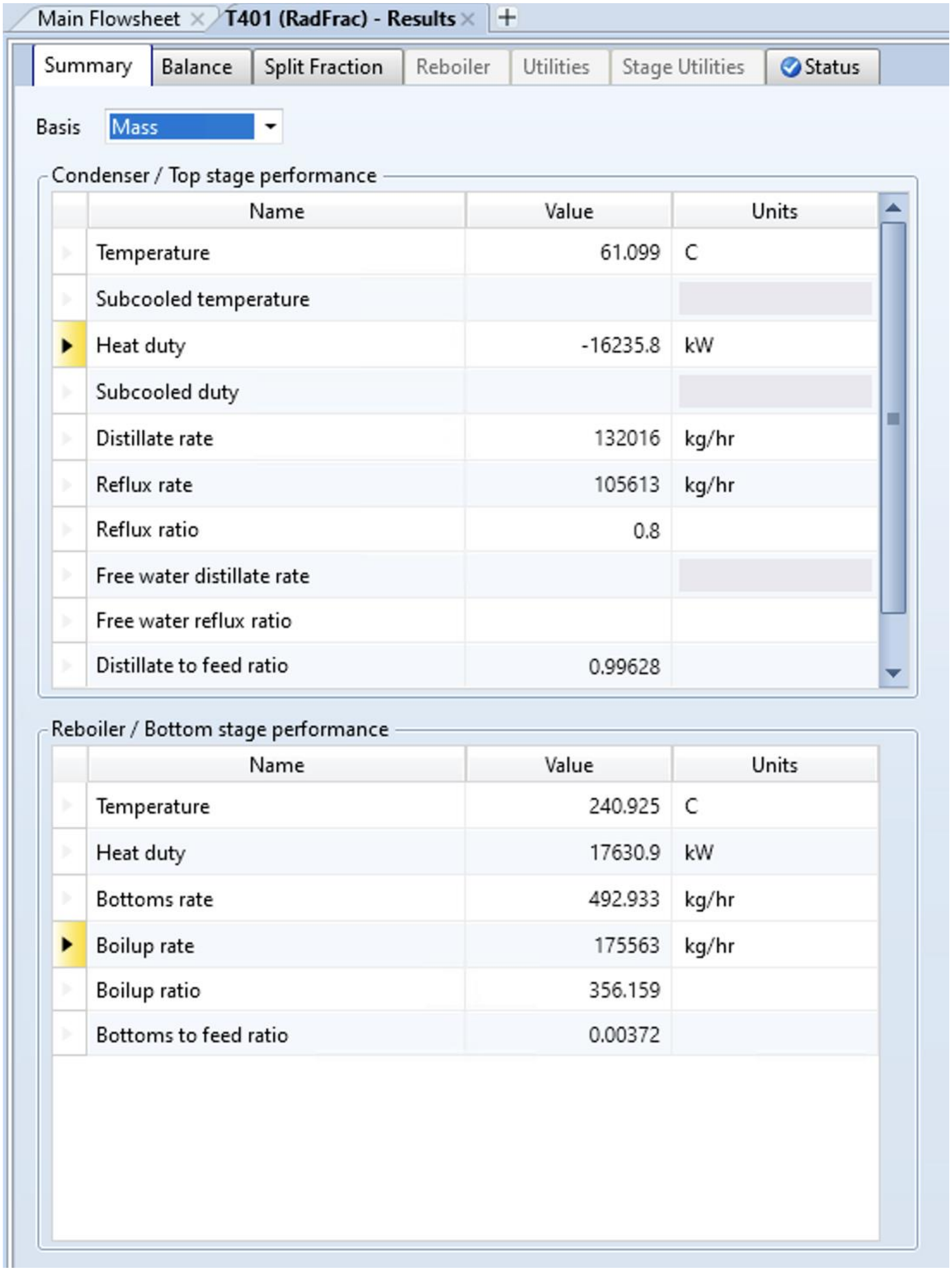
Condenser / Top stage performance

Name	Value	Units
Temperature	64.7371	C
Subcooled temperature		
Heat duty	-99013.1	kW
Subcooled duty		
Distillate rate	160500	kg/hr
Reflux rate	160500	kg/hr
Reflux ratio	1	
Free water distillate rate		
Free water reflux ratio		
Distillate to feed ratio	0.442	

Reboiler / Bottom stage performance

Name	Value	Units
Temperature	99.4611	C
Heat duty	123138	kW
Bottoms rate	202622	kg/hr
Boilup rate	199057	kg/hr
Boilup ratio	0.982405	
Bottoms to feed ratio	0.558	

Supplementary Figure 2. Summary of Condenser and Reboiler Properties for Distillation Column T-400



Supplementary Figure 3. Summary of Condenser and Reboiler Properties for Distillation Column T-401

Main Flowsheet | T400 (RadFrac) - Stream Results (Boundary)

Material | Heat | Load | Vol.% Curves | Wt. % Curves | Petroleum | Polymers | Solids

	Units	FEED	METH	WATER
+ Mole Flows	**kmol/hr**	**16259.3**	**5038.03**	**11221.3**
+ Mole Fractions				
− Mass Flows	**kg/hr**	**363122**	**160500**	**202622**
WATER	kg/hr	202748	1193.46	201555
METHANOL	kg/hr	160374	159307	1067.31
CHLOR-01	kg/hr	0	0	0
TRIOL-01	kg/hr	0	0	0
− Mass Fractions				
WATER		0.558347	0.00743589	0.994733
METHANOL		0.441653	0.992564	0.00526749
CHLOR-01		0	0	0
TRIOL-01		0	0	0

Supplementary Figure 4. Summary of Stream Mass Flow Rates and Mass Fractions for Distillation Column T-400

Main Flowsheet | T401 (RadFrac) - Stream Results (Boundary)

Material | Heat | Load | Vol.% Curves | Wt. % Curves | Petroleum | Polymers | Solids

	Units	FEED2	CHLORO	TRIOL
+ Mole Flows	**kmol/hr**	**1106.53**	**1105.87**	**0.656952**
+ Mole Fractions				
− Mass Flows	**kg/hr**	**132509**	**132016**	**492.933**
WATER	kg/hr	0	0	0
METHANOL	kg/hr	0	0	0
CHLOR-01	kg/hr	132030	132016	13.8321
TRIOL-01	kg/hr	479.101	2.33408e-123	479.101
− Mass Fractions				
WATER		0	0	0
METHANOL		0	0	0
CHLOR-01		0.996384	1	0.0280608
TRIOL-01		0.00361561	1.76803e-128	0.971939

Supplementary Figure 5. Summary of Stream Mass Flow Rates and Mass Fractions for Distillation Column T-401

```
+ + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + +
+ + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + + +
+ +                                                                           + +
+ +                    ASPEN PLUS CALCULATION REPORT                          + +
+ +                                                                           + +
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ASPEN PLUS IS A TRADEMARK OF ASPEN TECHNOLOGY, INC. 781/221-6400

HOTLINE:
U.S.A. 888/996-7100
EUROPE (44) 1189-226555

PLATFORM: WIN-X64
VERSION: 39.0 Build 116
INSTALLATION:

APRIL 18, 2022
MONDAY
12:56:18 A.M.

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```
ASPEN PLUS   PLAT: WIN-X64   VER: 39.0                   04/18/2022  PAGE 1
                            PHA SEPARATION TRAIN
                             RUN CONTROL SECTION

RUN CONTROL INFORMATION
-----------------------

THIS COPY OF ASPEN PLUS LICENSED TO UNIVERSITY OF PENNSYLVAN

TYPE OF RUN: NEW

INPUT FILE NAME: _4622gsl.inm

OUTPUT PROBLEM DATA FILE NAME: _4622gsl
LOCATED IN:


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

CALLING PROGRAM NAME:          apmain
LOCATED IN: C:\Program Files\AspenTech\Aspen Plus V12.1\Engine\\xeq

SIMULATION REQUESTED FOR ENTIRE FLOWSHEET

ASPEN PLUS   PLAT: WIN-X64   VER: 39.0                   04/18/2022  PAGE 2
                            PHA SEPARATION TRAIN
                              FLOWSHEET SECTION

FLOWSHEET CONNECTIVITY BY STREAMS
---------------------------------

  STREAM     SOURCE     DEST           STREAM     SOURCE     DEST
  FEED       ----       T400           FEED2      ----       T401
  METH       T400       ----           WATER      T400       ----
  CHLORO     T401       ----           TRIOL      T401       ----

FLOWSHEET CONNECTIVITY BY BLOCKS
--------------------------------

  BLOCK        INLETS                          OUTLETS
  T400         FEED                            METH WATER
  T401         FEED2                           CHLORO TRIOL

COMPUTATIONAL SEQUENCE
----------------------

SEQUENCE USED WAS:
   T401 T400

OVERALL FLOWSHEET BALANCE
-------------------------

                     ***  MASS AND ENERGY BALANCE  ***
                                  IN              OUT        RELATIVE DIFF.
   CONVENTIONAL COMPONENTS (KMOL/SEC)
      WATER                   3.12618         3.12618       -0.370541E-07
      METHANOL                1.39030         1.39030        0.833183E-07
      CHLOR-01               0.307220        0.307220       -0.271033E-14
      TRIOL-01               0.150301E-03    0.150301E-03    0.555461E-11
   TOTAL BALANCE
```

```
      MOLE(KMOL/SEC)           4.82385        4.82385         0.00000
      MASS(KG/SEC  )           137.675        137.675        0.118020E-07
      ENTHALPY(WATT    )      -0.126734E+10   -0.124182E+10   -0.201364E-01

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

ASPEN PLUS   PLAT: WIN-X64   VER: 39.0                  04/18/2022  PAGE 3
                             PHA SEPARATION TRAIN
                          PHYSICAL PROPERTIES SECTION

 COMPONENTS
 ----------

  ID       TYPE  ALIAS          NAME
   WATER    C     H2O            WATER
   METHANOL C     CH4O           METHANOL
   CHLOR-01 C     CHCL3          CHLOROFORM
   TRIOL-01 C     C57H104O6      TRIOLEIN

ASPEN PLUS   PLAT: WIN-X64   VER: 39.0                  04/18/2022  PAGE 4
                             PHA SEPARATION TRAIN
                              U-O-S BLOCK SECTION

 BLOCK:  T400     MODEL: RADFRAC
 -------------------------------
    INLETS   - FEED     STAGE  15
    OUTLETS  - METH     STAGE   1
               WATER    STAGE  30
   PROPERTY OPTION SET:   UNIFAC    UNIFAC / REDLICH-KWONG

                   ***  MASS AND ENERGY BALANCE  ***
                                   IN              OUT        RELATIVE DIFF.
    TOTAL BALANCE
      MOLE(KMOL/SEC)           4.51648        4.51648         0.00000
      MASS(KG/SEC  )           100.867        100.867        0.161087E-07
      ENTHALPY(WATT    )      -0.122576E+10   -0.120163E+10   -0.196814E-01

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


                        **********************
                        ****  INPUT DATA  ****
                        **********************

   ****   INPUT PARAMETERS   ****

    NUMBER OF STAGES                                      30
    ALGORITHM OPTION                                    STANDARD
    ABSORBER OPTION                                     NO
    INITIALIZATION OPTION                               STANDARD
    HYDRAULIC PARAMETER CALCULATIONS                    NO
    INSIDE LOOP CONVERGENCE METHOD                      BROYDEN
```

```
    DESIGN SPECIFICATION METHOD                         NESTED
    MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS                25
    MAXIMUM NO. OF INSIDE LOOP ITERATIONS                 10
    MAXIMUM NUMBER OF FLASH ITERATIONS                    30
    FLASH TOLERANCE                                        0.000100000
    OUTSIDE LOOP CONVERGENCE TOLERANCE                     0.000100000
```



```
 BLOCK:  T400     MODEL: RADFRAC (CONTINUED)

   ****   COL-SPECS   ****

    MOLAR VAPOR DIST / TOTAL DIST                          0.0
    MOLAR REFLUX RATIO                                     1.00000
    MASS DISTILLATE TO FEED RATIO                          0.44200

   ****    PROFILES   ****

    P-SPEC          STAGE   1  PRES, ATM                   1.00000

                         ******************
                         ****  RESULTS  ****
                         ******************


   ***   COMPONENT SPLIT FRACTIONS   ***

                            OUTLET STREAMS
                            --------------
                 METH         WATER
    COMPONENT:
    WATER       .58606E-02   .99414
    METHANOL    .99338       .66227E-02


   ***    SUMMARY OF KEY RESULTS    ***

    TOP STAGE TEMPERATURE          C                      64.7362
    BOTTOM STAGE TEMPERATURE       C                      99.4638
    TOP STAGE LIQUID FLOW          KMOL/SEC                1.39942
    BOTTOM STAGE LIQUID FLOW       KMOL/SEC                3.11706
    TOP STAGE VAPOR FLOW           KMOL/SEC                0.0
    BOILUP VAPOR FLOW              KMOL/SEC                3.01654
    MOLAR REFLUX RATIO                                     1.00000
    MOLAR BOILUP RATIO                                     0.96775
    CONDENSER DUTY (W/O SUBCOOL)   WATT                   -0.990120+08
    REBOILER DUTY                  WATT                    0.123136+09

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

    DEW POINT                       0.29235E-04  STAGE= 26
    BUBBLE POINT                    0.22183E-03  STAGE= 27
    COMPONENT MASS BALANCE          0.16489E-05  STAGE= 27 COMP=METHANOL
    ENERGY BALANCE                  0.20498E-04  STAGE= 25
```

BLOCK: T400   MODEL: RADFRAC (CONTINUED)

**** PROFILES ****

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

STAGE	TEMPERATURE C	PRESSURE ATM	ENTHALPY J/KMOL LIQUID	ENTHALPY J/KMOL VAPOR	HEAT DUTY WATT
1	64.736	1.0000	-0.23514E+09	-0.19946E+09	-.99012+08
2	65.033	1.0000	-0.23605E+09	-0.19977E+09	
13	74.856	1.0000	-0.26127E+09	-0.20923E+09	
14	75.871	1.0000	-0.26319E+09	-0.21017E+09	
15	76.664	1.0000	-0.26459E+09	-0.21090E+09	
16	76.664	1.0000	-0.26459E+09	-0.21090E+09	
17	76.663	1.0000	-0.26459E+09	-0.21090E+09	
29	97.797	1.0000	-0.27960E+09	-0.23577E+09	
30	99.464	1.0000	-0.27993E+09	-0.23843E+09	.12314+09

STAGE	FLOW RATE KMOL/SEC LIQUID	FLOW RATE KMOL/SEC VAPOR	FEED RATE KMOL/SEC LIQUID	FEED RATE KMOL/SEC VAPOR	FEED RATE KMOL/SEC MIXED	PRODUCT RATE KMOL/SEC LIQUID	PRODUCT RATE KMOL/SEC VAPOR
1	2.799	0.000				1.3994	
2	1.394	2.799					
13	1.254	2.664					
14	1.245	2.653					
15	6.302	2.644	4.5164				
16	6.302	3.185					
17	6.302	3.185					
29	6.134	3.002					
30	3.117	3.017				3.1170	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE KG/SEC LIQUID	FLOW RATE KG/SEC VAPOR	FEED RATE KG/SEC LIQUID	FEED RATE KG/SEC VAPOR	FEED RATE KG/SEC MIXED	PRODUCT RATE KG/SEC LIQUID	PRODUCT RATE KG/SEC VAPOR
1	89.17	0.000				44.5833	
2	44.02	89.17					
13	30.14	75.93					
14	29.20	74.72					
15	145.2	73.79	100.8672				
16	145.2	88.87					
17	145.2	88.87					
29	111.6	57.75					
30	56.28	55.29				56.2839	

BLOCK: T400   MODEL: RADFRAC (CONTINUED)

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

STAGE	WATER	METHANOL
1	0.13092E-01	0.98691
2	0.32279E-01	0.96772
13	0.57028	0.42972
14	0.61191	0.38809
15	0.64225	0.35775
16	0.64224	0.35776

17	0.64224	0.35776
29	0.98752	0.12483E-01
30	0.99705	0.29539E-02

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

STAGE	WATER	METHANOL
1	0.53061E-02	0.99469
2	0.13092E-01	0.98691
13	0.25259	0.74741
14	0.27637	0.72363
15	0.29500	0.70500
16	0.29499	0.70501
17	0.29497	0.70503
29	0.91257	0.87427E-01
30	0.97767	0.22330E-01

**** K-VALUES ****

STAGE	WATER	METHANOL
1	0.40531	1.0079
2	0.40561	1.0198
13	0.44295	1.7392
14	0.45167	1.8645
15	0.45934	1.9705
16	0.45933	1.9704
17	0.45932	1.9704
29	0.92411	7.0041
30	0.98057	7.5596

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

STAGE	WATER	METHANOL
1	0.74032E-02	0.99260
2	0.18409E-01	0.98159
13	0.42731	0.57269
14	0.46991	0.53009
15	0.50232	0.49768
16	0.50232	0.49768
17	0.50232	0.49768
29	0.97801	0.21989E-01
30	0.99476	0.52419E-02

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PHA SEPARATION TRAIN
U-O-S BLOCK SECTION

BLOCK: T400 MODEL: RADFRAC (CONTINUED)

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

STAGE	WATER	METHANOL
1	0.29902E-02	0.99701
2	0.74032E-02	0.99260
13	0.15967	0.84033
14	0.17677	0.82323
15	0.19046	0.80954
16	0.19045	0.80955
17	0.19044	0.80956
29	0.85441	0.14559
30	0.96096	0.39038E-01

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

```
                    ********************************

      *** DEFINITIONS ***

       MARANGONI INDEX = SIGMA - SIGMATO
       FLOW PARAM = (ML/MV)*SQRT(RHOV/RHOL)
       QR = QV*SQRT(RHOV/(RHOL-RHOV))
       F FACTOR = QV*SQRT(RHOV)
         WHERE:
         SIGMA IS THE SURFACE TENSION OF LIQUID FROM THE STAGE
         SIGMATO IS THE SURFACE TENSION OF LIQUID TO THE STAGE
         ML IS THE MASS FLOW OF LIQUID FROM THE STAGE
         MV IS THE MASS FLOW OF VAPOR TO THE STAGE
         RHOL IS THE MASS DENSITY OF LIQUID FROM THE STAGE
         RHOV IS THE MASS DENSITY OF VAPOR TO THE STAGE
         QV IS THE VOLUMETRIC FLOW RATE OF VAPOR TO THE STAGE
```

	TEMPERATURE C	
STAGE	LIQUID FROM	VAPOR TO
1	64.736	65.033
2	65.033	65.401
13	74.856	75.871
14	75.871	76.664
15	76.664	76.664
16	76.664	76.663
17	76.663	76.663
29	97.797	99.464
30	99.464	99.464

BLOCK: T400   MODEL: RADFRAC (CONTINUED)

	MASS FLOW KG/SEC		VOLUME FLOW CUM/SEC		MOLECULAR WEIGHT	
STAGE	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO
1	89.167	89.167	0.11972	76.612	31.859	31.859
2	44.020	88.603	0.59014E-01	76.540	31.589	31.724
13	30.139	74.722	0.37456E-01	75.119	24.043	28.166
14	29.204	73.787	0.35952E-01	75.055	23.459	27.904
15	145.15	88.869	0.17739	90.395	23.033	27.904
16	145.15	88.868	0.17739	90.393	23.034	27.905
17	145.15	88.867	0.17739	90.392	23.033	27.905
29	111.57	55.289	0.12204	91.565	18.190	18.329
30	56.284	0.0000	0.61356E-01	0.0000	18.057	

	DENSITY KG/CUM		VISCOSITY N-SEC/SQM		SURFACE TENSION N/M
STAGE	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM
1	744.77	1.1639	0.34523E-03	0.11068E-04	0.19473E-01
2	745.92	1.1576	0.34587E-03	0.11091E-04	0.20331E-01
13	804.65	0.99472	0.35021E-03	0.11713E-04	0.43688E-01
14	812.29	0.98311	0.34884E-03	0.11756E-04	0.45411E-01
15	818.27	0.98312	0.34755E-03	0.11756E-04	0.46653E-01
16	818.27	0.98312	0.34756E-03	0.11756E-04	0.46653E-01
17	818.27	0.98313	0.34756E-03	0.11756E-04	0.46653E-01

29	914.25	0.60382	0.28603E-03	0.12598E-04	0.58139E-01
30	917.33		0.28107E-03		0.58226E-01

STAGE	MARANGONI INDEX N/M	FLOW PARAM	QR CUM/SEC	REDUCED F-FACTOR (KG-CUM)**.5/SEC
1		0.39531E-01	3.0309	82.651
2	0.85792E-03	0.19572E-01	3.0176	82.351
13	0.22098E-02	0.14182E-01	2.6428	74.920
14	0.17233E-02	0.13769E-01	2.6127	74.418
15	-.77682E-02	0.56615E-01	3.1352	89.629
16	-.56182E-07	0.56615E-01	3.1351	89.628
17	0.15853E-06	0.56616E-01	3.1351	89.626
29	0.51651E-03	0.51861E-01	2.3539	71.151
30	0.87127E-04		0.0000	0.0000

BLOCK: T400 MODEL: RADFRAC (CONTINUED)

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

   *******************
   *** SECTION   1 ***
   *******************

   STARTING STAGE NUMBER                                        2
   ENDING STAGE NUMBER                                         29
   FLOODING CALCULATION METHOD                            GLITSCH6

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

   TRAY SPECIFICATIONS
   -------------------
   TRAY TYPE                                              SIEVE
   NUMBER OF PASSES                                             2
   TRAY SPACING                    METER                  0.45720


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

   STAGE WITH MAXIMUM DIAMETER                                 15
   COLUMN DIAMETER                 METER                  8.60854
   DC AREA/COLUMN AREA                                    0.17500
   SIDE DOWNCOMER VELOCITY         M/SEC                  0.034831
   FLOW PATH LENGTH PER PANEL      METER                  3.12817
   SIDE DOWNCOMER WIDTH            METER                  0.83769
   SIDE WEIR LENGTH                METER                  5.10277
   CENTER DOWNCOMER WIDTH          METER                  0.67682
```

CENTER WEIR LENGTH	METER	8.58189
OFF-CENTER DOWNCOMER WIDTH	METER	0.0
OFF-CENTER SHORT WEIR LENGTH	METER	MISSING
OFF-CENTER LONG WEIR LENGTH	METER	MISSING
TRAY CENTER TO OCDC CENTER	METER	0.0

**** SIZING PROFILES ****

STAGE	DIAMETER	TOTAL AREA	ACTIVE AREA PER PANEL	SIDE DC AREA PER PANEL
	METER	SQM	SQM	SQM
2	8.6085	58.203	23.281	2.5464
3	8.6085	58.203	23.281	2.5464
4	8.6085	58.203	23.281	2.5464
5	8.6085	58.203	23.281	2.5464
6	8.6085	58.203	23.281	2.5464
7	8.6085	58.203	23.281	2.5464
8	8.6085	58.203	23.281	2.5464
9	8.6085	58.203	23.281	2.5464
10	8.6085	58.203	23.281	2.5464

BLOCK: T400 MODEL: RADFRAC (CONTINUED)

STAGE	DIAMETER	TOTAL AREA	ACTIVE AREA PER PANEL	SIDE DC AREA PER PANEL
	METER	SQM	SQM	SQM
11	8.6085	58.203	23.281	2.5464
12	8.6085	58.203	23.281	2.5464
13	8.6085	58.203	23.281	2.5464
14	8.6085	58.203	23.281	2.5464
15	8.6085	58.203	23.281	2.5464
16	8.6085	58.203	23.281	2.5464
17	8.6085	58.203	23.281	2.5464
18	8.6085	58.203	23.281	2.5464
19	8.6085	58.203	23.281	2.5464
20	8.6085	58.203	23.281	2.5464
21	8.6085	58.203	23.281	2.5464
22	8.6085	58.203	23.281	2.5464
23	8.6085	58.203	23.281	2.5464
24	8.6085	58.203	23.281	2.5464
25	8.6085	58.203	23.281	2.5464
26	8.6085	58.203	23.281	2.5464
27	8.6085	58.203	23.281	2.5464
28	8.6085	58.203	23.281	2.5464
29	8.6085	58.203	23.281	2.5464

**** ADDITIONAL SIZING PROFILES ****

STAGE	FLOODING FACTOR	PRES. DROP	DC BACKUP	DC BACKUP/ (TSPC+WHT)
		N/SQM	METER	
2	65.42	490.2	0.1549	31.27
3	65.08	488.8	0.1540	31.09
4	64.66	487.1	0.1530	30.89
5	64.16	485.2	0.1518	30.64
6	63.56	483.0	0.1503	30.35
7	62.86	480.6	0.1487	30.02

8	62.06	478.1	0.1468	29.64
9	61.16	475.7	0.1448	29.23
10	60.21	473.5	0.1427	28.81
11	59.24	471.7	0.1406	28.39
12	58.32	470.4	0.1387	28.00
13	57.52	469.7	0.1371	27.67
14	56.88	469.4	0.1358	27.41
15	80.00	658.2	0.2582	52.12
16	80.00	658.2	0.2581	52.12
17	80.00	658.2	0.2581	52.12
18	80.00	658.2	0.2581	52.12
19	79.99	658.2	0.2581	52.11
20	79.98	658.1	0.2581	52.11
21	79.96	657.9	0.2580	52.08
22	79.88	657.4	0.2576	52.01
23	79.67	656.0	0.2566	51.80
24	79.05	651.9	0.2537	51.21

BLOCK: T400 MODEL: RADFRAC (CONTINUED)

STAGE	FLOODING FACTOR	PRES. DROP N/SQM	DC BACKUP METER	DC BACKUP/ (TSPC+WHT)
25	77.41	641.3	0.2461	49.68
26	73.70	619.6	0.2301	46.45
27	68.46	593.7	0.2096	42.33
28	65.11	580.5	0.1973	39.83
29	64.09	577.1	0.1932	39.00

STAGE	HEIGHT OVER WEIR METER	DC REL FROTH DENS	TR LIQ REL FROTH DENS	FRA APPR TO SYS LIMIT
2	0.4725E-01	0.6068	0.2289	32.77
3	0.4659E-01	0.6068	0.2296	32.20
4	0.4581E-01	0.6069	0.2305	31.54
5	0.4487E-01	0.6069	0.2315	30.80
6	0.4376E-01	0.6070	0.2327	29.97
7	0.4247E-01	0.6070	0.2342	29.09
8	0.4102E-01	0.6071	0.2358	28.15
9	0.3944E-01	0.6072	0.2376	27.21
10	0.3777E-01	0.6073	0.2396	26.28
11	0.3613E-01	0.6074	0.2415	25.43
12	0.3462E-01	0.6075	0.2433	24.68
13	0.3333E-01	0.6076	0.2448	24.08
14	0.3232E-01	0.6077	0.2460	23.63
15	0.1027	0.6078	0.2161	28.26
16	0.1027	0.6078	0.2161	28.26
17	0.1027	0.6078	0.2161	28.26
18	0.1027	0.6078	0.2161	28.26
19	0.1027	0.6078	0.2161	28.26
20	0.1027	0.6078	0.2161	28.25
21	0.1026	0.6078	0.2162	28.24
22	0.1025	0.6078	0.2163	28.20
23	0.1021	0.6078	0.2167	28.08
24	0.1009	0.6078	0.2179	27.76
25	0.9762E-01	0.6078	0.2211	26.90
26	0.9044E-01	0.6079	0.2290	25.02
27	0.8044E-01	0.6081	0.2417	22.51
28	0.7390E-01	0.6081	0.2510	20.98

```
 29    0.7167E-01  0.6082      0.2541       20.51

BLOCK:  T401     MODEL: RADFRAC
-------------------------------
   INLETS   - FEED2    STAGE   7
   OUTLETS  - CHLORO   STAGE   1
              TRIOL    STAGE  15
  PROPERTY OPTION SET:   UNIFAC    UNIFAC / REDLICH-KWONG
```



```
BLOCK:  T401     MODEL: RADFRAC (CONTINUED)

                     ***  MASS AND ENERGY BALANCE  ***
                                   IN              OUT        RELATIVE DIFF.
   TOTAL BALANCE
      MOLE(KMOL/SEC)           0.307370        0.307370         0.00000
      MASS(KG/SEC  )            36.8081         36.8081        0.173736E-13
      ENTHALPY(WATT    )      -0.415836E+08   -0.401885E+08   -0.335492E-01

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


                        **********************
                        ****  INPUT DATA  ****
                        **********************

  ****   INPUT PARAMETERS   ****

   NUMBER OF STAGES                                        15
   ALGORITHM OPTION                                      STANDARD
   ABSORBER OPTION                                       NO
   INITIALIZATION OPTION                                 STANDARD
   HYDRAULIC PARAMETER CALCULATIONS                      NO
   INSIDE LOOP CONVERGENCE METHOD                        BROYDEN
   DESIGN SPECIFICATION METHOD                           NESTED
   MAXIMUM NO. OF OUTSIDE LOOP ITERATIONS                  25
   MAXIMUM NO. OF INSIDE LOOP ITERATIONS                   10
   MAXIMUM NUMBER OF FLASH ITERATIONS                      30
   FLASH TOLERANCE                                          0.000100000
   OUTSIDE LOOP CONVERGENCE TOLERANCE                       0.000100000

  ****   COL-SPECS   ****

   MOLAR VAPOR DIST / TOTAL DIST                            0.0
   MASS REFLUX RATIO                                        0.80000
   MASS DISTILLATE TO FEED RATIO                            0.99628
```

BLOCK: T401 MODEL: RADFRAC (CONTINUED)

**** PROFILES ****

P-SPEC STAGE 1 PRES, ATM 1.00000

****
**** RESULTS ****
****

*** COMPONENT SPLIT FRACTIONS ***

	OUTLET STREAMS	
	CHLORO	TRIOL
COMPONENT:		
CHLOR-01	.99990	.10477E-03
TRIOL-01	0.0000	1.0000

*** SUMMARY OF KEY RESULTS ***

TOP STAGE TEMPERATURE	C	61.0990
BOTTOM STAGE TEMPERATURE	C	240.933
TOP STAGE LIQUID FLOW	KMOL/SEC	0.24575
BOTTOM STAGE LIQUID FLOW	KMOL/SEC	0.00018249
TOP STAGE VAPOR FLOW	KMOL/SEC	0.0
BOILUP VAPOR FLOW	KMOL/SEC	0.40854
MOLAR REFLUX RATIO		0.80000
MOLAR BOILUP RATIO		2,238.76
CONDENSER DUTY (W/O SUBCOOL)	WATT	-0.162358+08
REBOILER DUTY	WATT	0.176309+08

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

DEW POINT	0.43661E-03	STAGE= 15	
BUBBLE POINT	0.15068E-06	STAGE= 15	
COMPONENT MASS BALANCE	0.11476E-06	STAGE= 14	COMP=TRIOL-01
ENERGY BALANCE	0.62348E-07	STAGE= 15	

BLOCK: T401 MODEL: RADFRAC (CONTINUED)

**** PROFILES ****

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

STAGE	TEMPERATURE C	PRESSURE ATM	ENTHALPY J/KMOL LIQUID	ENTHALPY J/KMOL VAPOR	HEAT DUTY WATT
1	61.099	1.0000	-0.13001E+09	-0.10064E+09	-.16236+08
2	61.099	1.0000	-0.13001E+09	-0.10064E+09	

6	61.099	1.0000	-0.13001E+09	-0.10064E+09	
7	61.107	1.0000	-0.13048E+09	-0.10064E+09	
8	61.107	1.0000	-0.13048E+09	-0.10064E+09	
9	61.107	1.0000	-0.13048E+09	-0.10064E+09	
14	61.111	1.0000	-0.13070E+09	-0.10064E+09	
15	240.93	1.0000	-0.13827E+10	-0.86982E+08	.17631+08

STAGE	FLOW RATE KMOL/SEC		FEED RATE KMOL/SEC			PRODUCT RATE KMOL/SEC	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	0.5529	0.000				0.3071	
2	0.2457	0.5529					
6	0.2457	0.5529					
7	0.5988	0.5529	0.3073				
8	0.5988	0.5986					
9	0.5988	0.5986					
14	0.4087	0.5986					
15	0.1825E-03	0.4085				.18249-03	

**** MASS FLOW PROFILES ****

STAGE	FLOW RATE KG/SEC		FEED RATE KG/SEC			PRODUCT RATE KG/SEC	
	LIQUID	VAPOR	LIQUID	VAPOR	MIXED	LIQUID	VAPOR
1	66.01	0.000				36.6711	
2	29.34	66.01					
6	29.34	66.01					
7	71.60	66.01	36.8080				
8	71.60	71.46					
9	71.60	71.46					
14	48.91	71.46					
15	0.1369	48.77				0.1369	

BLOCK: T401 MODEL: RADFRAC (CONTINUED)

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

STAGE	CHLOR-01	TRIOL-01
1	1.0000	0.23823-128
2	1.0000	0.32410-107
6	1.0000	0.43323E-24
7	0.99975	0.25100E-03
8	0.99975	0.25100E-03
9	0.99975	0.25100E-03
14	0.99963	0.36823E-03
15	0.17637	0.82363

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

STAGE	CHLOR-01	TRIOL-01
1	1.0000	0.17511-149
2	1.0000	0.23823-128
6	1.0000	0.31844E-45
7	1.0000	0.19254E-24
8	1.0000	0.19254E-24
9	1.0000	0.19254E-24
14	1.0000	0.28814E-24
15	1.0000	0.50238E-06

**** K-VALUES ****

STAGE	CHLOR-01	TRIOL-01

1	1.0000	0.73504E-21
2	1.0000	0.73504E-21
6	1.0000	0.73504E-21
7	1.0003	0.76709E-21
8	1.0003	0.76709E-21
9	1.0003	0.76709E-21
14	1.0004	0.78249E-21
15	5.6698	0.61029E-06

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

STAGE	CHLOR-01	TRIOL-01
1	1.0000	0.17670-127
2	1.0000	0.24040-106
6	1.0000	0.32134E-23
7	0.99814	0.18587E-02
8	0.99814	0.18587E-02
9	0.99814	0.18587E-02
14	0.99728	0.27248E-02
15	0.28061E-01	0.97194

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

STAGE	CHLOR-01	TRIOL-01
1	1.0000	0.12988-148
2	1.0000	0.17670-127
6	1.0000	0.23619E-44
7	1.0000	0.14281E-23
8	1.0000	0.14281E-23
9	1.0000	0.14281E-23
14	1.0000	0.21372E-23
15	1.0000	0.37263E-05

BLOCK: T401 MODEL: RADFRAC (CONTINUED)

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

*** DEFINITIONS ***

MARANGONI INDEX = SIGMA - SIGMATO
FLOW PARAM = (ML/MV)*SQRT(RHOV/RHOL)
QR = QV*SQRT(RHOV/(RHOL-RHOV))
F FACTOR = QV*SQRT(RHOV)
WHERE:
SIGMA IS THE SURFACE TENSION OF LIQUID FROM THE STAGE
SIGMATO IS THE SURFACE TENSION OF LIQUID TO THE STAGE
ML IS THE MASS FLOW OF LIQUID FROM THE STAGE
MV IS THE MASS FLOW OF VAPOR TO THE STAGE
RHOL IS THE MASS DENSITY OF LIQUID FROM THE STAGE
RHOV IS THE MASS DENSITY OF VAPOR TO THE STAGE
QV IS THE VOLUMETRIC FLOW RATE OF VAPOR TO THE STAGE

	TEMPERATURE C	
STAGE	LIQUID FROM	VAPOR TO
1	61.099	61.099

2	61.099	61.099
6	61.099	61.107
7	61.107	61.107
8	61.107	61.107
9	61.107	61.107
14	61.111	240.93
15	240.93	240.93

	MASS FLOW KG/SEC		VOLUME FLOW CUM/SEC		MOLECULAR WEIGHT	
STAGE	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO
1	66.008	66.008	0.46751E-01	14.805	119.38	119.38
2	29.337	66.008	0.20778E-01	14.805	119.38	119.38
6	29.336	66.007	0.20777E-01	14.806	119.38	119.38
7	71.599	71.462	0.51244E-01	16.029	119.57	119.38
8	71.599	71.462	0.51244E-01	16.029	119.57	119.38
9	71.599	71.462	0.51244E-01	16.029	119.57	119.38
14	48.908	48.771	0.35173E-01	17.110	119.66	119.38
15	0.13693	0.0000	0.23509E-03	0.0000	750.33	

BLOCK: T401 MODEL: RADFRAC (CONTINUED)

	DENSITY KG/CUM		VISCOSITY N-SEC/SQM		SURFACE TENSION N/M
STAGE	LIQUID FROM	VAPOR TO	LIQUID FROM	VAPOR TO	LIQUID FROM
1	1411.9	4.4583	0.39172E-03	0.11584E-04	0.21901E-01
2	1411.9	4.4583	0.39172E-03	0.11584E-04	0.21901E-01
6	1411.9	4.4582	0.39172E-03	0.11584E-04	0.21901E-01
7	1397.2	4.4582	0.39207E-03	0.11584E-04	0.21901E-01
8	1397.2	4.4582	0.39207E-03	0.11584E-04	0.21901E-01
9	1397.2	4.4582	0.39207E-03	0.11584E-04	0.21901E-01
14	1390.5	2.8504	0.39224E-03	0.17437E-04	0.21901E-01
15	582.44		0.53404E-03		0.11590E-01

STAGE	MARANGONI INDEX N/M	FLOW PARAM	QR CUM/SEC	REDUCED F-FACTOR (KG-CUM)**.5/SEC
1		0.56193E-01	0.83329	31.261
2	-.20817E-16	0.24975E-01	0.83329	31.261
6	-.48572E-16	0.24974E-01	0.83328	31.261
7	-.25586E-02	0.56595E-01	0.90689	33.845
8	-.25491E-12	0.56595E-01	0.90689	33.845
9	-.25833E-12	0.56595E-01	0.90689	33.845
14	-.23502E-07	0.45403E-01	0.77548	28.888
15	-.10311E-01		0.0000	0.0000

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

****
*** SECTION 1 ***
****

STARTING STAGE NUMBER		2
ENDING STAGE NUMBER		14
FLOODING CALCULATION METHOD		GLITSCH6

DESIGN PARAMETERS

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

BLOCK: T401 MODEL: RADFRAC (CONTINUED)

TRAY SPECIFICATIONS

TRAY TYPE		SIEVE
NUMBER OF PASSES		1
TRAY SPACING	METER	0.45720

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

STAGE WITH MAXIMUM DIAMETER		7
COLUMN DIAMETER	METER	4.22173
DC AREA/COLUMN AREA		0.20159
DOWNCOMER VELOCITY	M/SEC	0.036318
FLOW PATH LENGTH PER PANEL	METER	2.89327
SIDE DOWNCOMER WIDTH	METER	0.66423
SIDE WEIR LENGTH	METER	3.07441
CENTER DOWNCOMER WIDTH	METER	0.0
CENTER WEIR LENGTH	METER	MISSING
OFF-CENTER DOWNCOMER WIDTH	METER	0.0
OFF-CENTER SHORT WEIR LENGTH	METER	MISSING
OFF-CENTER LONG WEIR LENGTH	METER	MISSING
TRAY CENTER TO OCDC CENTER	METER	0.0

**** SIZING PROFILES ****

STAGE	DIAMETER METER	TOTAL AREA SQM	ACTIVE AREA SQM	SIDE DC AREA SQM
2	4.2217	13.998	11.176	1.4110
3	4.2217	13.998	11.176	1.4110
4	4.2217	13.998	11.176	1.4110
5	4.2217	13.998	11.176	1.4110
6	4.2217	13.998	11.176	1.4110
7	4.2217	13.998	11.176	1.4110
8	4.2217	13.998	11.176	1.4110
9	4.2217	13.998	11.176	1.4110
10	4.2217	13.998	11.176	1.4110
11	4.2217	13.998	11.176	1.4110
12	4.2217	13.998	11.176	1.4110
13	4.2217	13.998	11.176	1.4110
14	4.2217	13.998	11.176	1.4110

**** ADDITIONAL SIZING PROFILES ****

STAGE	FLOODING FACTOR	PRES. DROP N/SQM	DC BACKUP METER	DC BACKUP/ (TSPC+WHT)
2	66.14	1109.	0.1877	37.90
3	66.14	1109.	0.1877	37.90
4	66.14	1109.	0.1877	37.90
5	66.14	1109.	0.1877	37.90
6	66.14	1109.	0.1877	37.90
7	80.12	1343.	0.3285	66.32
8	80.12	1343.	0.3285	66.32
9	80.12	1343.	0.3285	66.32
10	80.12	1343.	0.3285	66.32
11	80.12	1343.	0.3285	66.32
12	80.12	1343.	0.3285	66.32
13	80.12	1343.	0.3285	66.32

BLOCK: T401   MODEL: RADFRAC (CONTINUED)

STAGE	FLOODING FACTOR	PRES. DROP N/SQM	DC BACKUP METER	DC BACKUP/ (TSPC+WHT)
14	65.87	1079.	0.2334	47.13

STAGE	HEIGHT OVER WEIR METER	DC REL FROTH DENS	TR LIQ REL FROTH DENS	FRA APPR TO SYS LIMIT
2	0.7839E-01	0.6083	0.1764	43.88
3	0.7839E-01	0.6083	0.1764	43.88
4	0.7839E-01	0.6083	0.1764	43.88
5	0.7839E-01	0.6083	0.1764	43.88
6	0.7839E-01	0.6083	0.1764	43.88
7	0.1520	0.6083	0.1713	47.75
8	0.1520	0.6083	0.1713	47.75
9	0.1520	0.6083	0.1713	47.75
10	0.1520	0.6083	0.1713	47.75
11	0.1520	0.6083	0.1713	47.75
12	0.1520	0.6083	0.1713	47.75
13	0.1520	0.6083	0.1713	47.75
14	0.1107	0.6083	0.1825	40.43

CHLORO FEED FEED2 METH TRIOL

STREAM ID	CHLORO	FEED	FEED2	METH	TRIOL
FROM :	T401	----	----	T400	T401
TO :	----	T400	T401	----	----
SUBSTREAM: MIXED					
PHASE:	LIQUID	LIQUID	LIQUID	LIQUID	LIQUID
COMPONENTS: KMOL/SEC					
WATER	0.0	3.1262	0.0	1.8321-02	0.0
METHANOL	0.0	1.3903	0.0	1.3811	0.0

```
  CHLOR-01              0.3072     0.0        0.3072     0.0      3.2186-05
  TRIOL-01              0.0        0.0      1.5030-04    0.0      1.5030-04
COMPONENTS: KG/SEC
  WATER                 0.0       56.3189     0.0        0.3301     0.0
  METHANOL              0.0       44.5483     0.0       44.2532     0.0
  CHLOR-01             36.6711     0.0       36.6750     0.0      3.8423-03
  TRIOL-01              0.0        0.0        0.1331     0.0        0.1331
TOTAL FLOW:
  KMOL/SEC              0.3072     4.5165     0.3074     1.3994   1.8249-04
  KG/SEC               36.6711   100.8672    36.8081    44.5833     0.1369
  CUM/SEC             2.5973-02    0.1136   2.5376-02  5.9862-02  2.3509-04
STATE VARIABLES:
  TEMP   C             61.0990    25.0000    25.0000    64.7362   240.9328
  PRES   ATM            1.0000     1.0000     1.0000     1.0000     1.0000
  VFRAC                 0.0        0.0        0.0        0.0        0.0
  LFRAC                 1.0000     1.0000     1.0000     1.0000     1.0000
  SFRAC                 0.0        0.0        0.0        0.0        0.0
ENTHALPY:
  J/KMOL             -1.3001+08 -2.7140+08 -1.3529+08 -2.3514+08 -1.3827+09
  J/KG               -1.0890+06 -1.2152+07 -1.1297+06 -7.3809+06 -1.8427+06
  WATT               -3.9936+07 -1.2258+09 -4.1584+07 -3.2906+08 -2.5232+05
ENTROPY:
  J/KMOL-K           -1.9049+05 -1.8352+05 -2.0671+05 -2.2700+05 -3.7488+06
  J/KG-K             -1595.7080 -8217.3398 -1726.1322 -7125.1984 -4996.1454
DENSITY:
  KMOL/CUM             11.8272    39.7434    12.1127    23.3774     0.7762
  KG/CUM             1411.8963   887.5958  1450.5110   744.7704   582.4449
AVG MW                119.3770    22.3332   119.7516    31.8585   750.3340
```



```
WATER
-----

STREAM ID               WATER
FROM :                  T400
TO   :                  ----

SUBSTREAM: MIXED
PHASE:                  LIQUID
COMPONENTS: KMOL/SEC
  WATER                 3.1079
  METHANOL            9.2076-03
  CHLOR-01              0.0
  TRIOL-01              0.0
COMPONENTS: KG/SEC
  WATER                55.9889
  METHANOL              0.2950
  CHLOR-01              0.0
  TRIOL-01              0.0
TOTAL FLOW:
  KMOL/SEC              3.1171
  KG/SEC               56.2839
  CUM/SEC             6.1356-02
STATE VARIABLES:
  TEMP   C             99.4638
  PRES   ATM            1.0000
  VFRAC                 0.0
  LFRAC                 1.0000
  SFRAC                 0.0
ENTHALPY:
```

```
   J/KMOL            -2.7993+08
   J/KG              -1.5503+07
   WATT              -8.7257+08
 ENTROPY:
   J/KMOL-K          -1.4618+05
   J/KG-K            -8095.3362
 DENSITY:
   KMOL/CUM             50.8028
   KG/CUM              917.3316
 AVG MW                 18.0567
```


FLASH CURVE TABLE: BINRY-1

```
   PROPERTIES ALONG A FLASH CURVE FOR THE MIXTURE:  (KMOL/SEC    )
       WATER     1.000     , TRIOL-01  1.000     ,

   STATE SPECIFICATIONS:
       VAPOR FRACTION:     0.000

   VARIED VARIABLE(S):    PRES      MOLEFRAC

   PROPERTY SET(S):       $PS-TXY

   3 PHASE PV FLASHES WERE PERFORMED.

   PROPERTY OPTION SET:   UNIFAC    UNIFAC / REDLICH-KWONG
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FLASH CURVE TABLE: BINRY-1 (CONTINUED)

PRES ATM	MOLEFRAC WATER	TEMP TOTAL C	KVL TOTAL WATER	KVL TOTAL TRIOL-01	GAMMA LIQUID 1 WATER
1.0000	0.0	623.5040	151.1510	1.0000	1.1725
1.0000	2.0000-02	198.2999	50.0000	1.4097-08	3.5964
1.0000	4.0000-02	159.8421	25.0000	2.1555-10	4.2374
1.0000	6.0000-02	141.0458	16.6667	1.9523-11	4.6185
1.0000	8.0000-02	128.9868	12.5000	3.6109-12	4.8904
1.0000	0.1000	120.2678	10.0000	9.8475-13	5.1006
1.0000	0.1200	113.5208	8.3333	3.4307-13	5.2703
1.0000	0.1400	108.0665	7.1429	1.4152-13	5.4108
1.0000	0.1600	103.5208	6.2500	6.6084-14	5.5289
1.0000	0.1800	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.2000	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.2200	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.2400	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.2600	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.2800	100.0178	5.6195	3.6196-14	5.6195

1.0000	0.3000	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.3200	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.3400	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.3600	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.3800	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.4000	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.4200	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.4400	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.4600	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.4800	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.5000	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.5200	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.5400	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.5600	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.5800	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.6000	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.6200	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.6400	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.6600	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.6800	100.0178	5.6195	3.6196-14	5.6195

FLASH CURVE TABLE: BINRY-1 (CONTINUED)

PRES ATM	MOLEFRAC WATER	TEMP TOTAL C	KVL TOTAL WATER	KVL TOTAL TRIOL-01	GAMMA LIQUID 1 WATER
1.0000	0.7000	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.7200	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.7400	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.7600	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.7800	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.8000	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.8200	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.8400	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.8600	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.8800	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.9000	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.9200	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.9400	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.9600	100.0178	5.6195	3.6196-14	5.6195
1.0000	0.9800	100.0178	5.6195	3.6196-14	5.6195
1.0000	1.0000	100.0178	1.0000	1.5090+08	1.0000

PRES	MOLEFRAC	GAMMA	GAMMA	GAMMA	KVL2

		LIQUID 1	LIQUID 2	LIQUID 2	TOTAL
	WATER	TRIOL-01	WATER	TRIOL-01	WATER
ATM					
1.0000	0.0	1.0000	MISSING	MISSING	MISSING
1.0000	2.0000-02	0.9999	MISSING	MISSING	MISSING
1.0000	4.0000-02	0.9998	MISSING	MISSING	MISSING
1.0000	6.0000-02	0.9997	MISSING	MISSING	MISSING
1.0000	8.0000-02	0.9995	MISSING	MISSING	MISSING
1.0000	0.1000	0.9994	MISSING	MISSING	MISSING
1.0000	0.1200	0.9992	MISSING	MISSING	MISSING
1.0000	0.1400	0.9992	MISSING	MISSING	MISSING
1.0000	0.1600	0.9992	MISSING	MISSING	MISSING
1.0000	0.1800	0.9993	1.0000	4.1661+21	1.0000

FLASH CURVE TABLE: BINRY-1 (CONTINUED)

PRES	MOLEFRAC	GAMMA	GAMMA	GAMMA	KVL2
		LIQUID 1	LIQUID 2	LIQUID 2	TOTAL
	WATER	TRIOL-01	WATER	TRIOL-01	WATER
ATM					
1.0000	0.2000	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.2200	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.2400	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.2600	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.2800	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.3000	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.3200	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.3400	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.3600	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.3800	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.4000	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.4200	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.4400	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.4600	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.4800	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.5000	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.5200	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.5400	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.5600	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.5800	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.6000	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.6200	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.6400	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.6600	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.6800	0.9993	1.0000	4.1661+21	1.0000

1.0000	0.7000	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.7200	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.7400	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.7600	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.7800	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.8000	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.8200	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.8400	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.8600	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.8800	0.9993	1.0000	4.1661+21	1.0000

FLASH CURVE TABLE: BINRY-1 (CONTINUED)

PRES ATM	MOLEFRAC WATER	GAMMA LIQUID 1 TRIOL-01	GAMMA LIQUID 2 WATER	GAMMA LIQUID 2 TRIOL-01	KVL2 TOTAL WATER
1.0000	0.9000	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.9200	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.9400	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.9600	0.9993	1.0000	4.1661+21	1.0000
1.0000	0.9800	0.9993	1.0000	4.1661+21	1.0000
1.0000	1.0000	4.1661+21	MISSING	MISSING	MISSING

PRES ATM	MOLEFRAC WATER	KVL2 TOTAL TRIOL-01	BETA TOTAL	MOLEFRAC VAPOR WATER	MOLEFRAC VAPOR TRIOL-01
1.0000	0.0	MISSING	1.0000	0.0	1.0000
1.0000	2.0000-02	MISSING	1.0000	1.0000	1.3815-08
1.0000	4.0000-02	MISSING	1.0000	1.0000	2.0693-10
1.0000	6.0000-02	MISSING	1.0000	1.0000	1.8351-11
1.0000	8.0000-02	MISSING	1.0000	1.0000	3.3221-12
1.0000	0.1000	MISSING	1.0000	1.0000	8.8627-13
1.0000	0.1200	MISSING	1.0000	1.0000	3.0190-13
1.0000	0.1400	MISSING	1.0000	1.0000	1.2171-13
1.0000	0.1600	MISSING	1.0000	1.0000	5.5511-14
1.0000	0.1800	1.5090+08	0.9975	1.0000	2.9755-14
1.0000	0.2000	1.5090+08	0.9732	1.0000	2.9755-14
1.0000	0.2200	1.5090+08	0.9488	1.0000	2.9755-14
1.0000	0.2400	1.5090+08	0.9245	1.0000	2.9755-14
1.0000	0.2600	1.5090+08	0.9002	1.0000	2.9755-14
1.0000	0.2800	1.5090+08	0.8759	1.0000	2.9755-14
1.0000	0.3000	1.5090+08	0.8515	1.0000	2.9755-14

1.0000	0.3200	1.5090+08	0.8272	1.0000	2.9755-14
1.0000	0.3400	1.5090+08	0.8029	1.0000	2.9755-14
1.0000	0.3600	1.5090+08	0.7785	1.0000	2.9755-14
1.0000	0.3800	1.5090+08	0.7542	1.0000	2.9755-14

FLASH CURVE TABLE: BINRY-1 (CONTINUED)

PRES ATM	MOLEFRAC WATER	KVL2 TOTAL TRIOL-01	BETA TOTAL	MOLEFRAC VAPOR WATER	MOLEFRAC VAPOR TRIOL-01
1.0000	0.4000	1.5090+08	0.7299	1.0000	2.9755-14
1.0000	0.4200	1.5090+08	0.7056	1.0000	2.9755-14
1.0000	0.4400	1.5090+08	0.6812	1.0000	2.9755-14
1.0000	0.4600	1.5090+08	0.6569	1.0000	2.9755-14
1.0000	0.4800	1.5090+08	0.6326	1.0000	2.9755-14
1.0000	0.5000	1.5090+08	0.6082	1.0000	2.9755-14
1.0000	0.5200	1.5090+08	0.5839	1.0000	2.9755-14
1.0000	0.5400	1.5090+08	0.5596	1.0000	2.9755-14
1.0000	0.5600	1.5090+08	0.5352	1.0000	2.9755-14
1.0000	0.5800	1.5090+08	0.5109	1.0000	2.9755-14
1.0000	0.6000	1.5090+08	0.4866	1.0000	2.9755-14
1.0000	0.6200	1.5090+08	0.4623	1.0000	2.9755-14
1.0000	0.6400	1.5090+08	0.4379	1.0000	2.9755-14
1.0000	0.6600	1.5090+08	0.4136	1.0000	2.9755-14
1.0000	0.6800	1.5090+08	0.3893	1.0000	2.9755-14
1.0000	0.7000	1.5090+08	0.3649	1.0000	2.9755-14
1.0000	0.7200	1.5090+08	0.3406	1.0000	2.9755-14
1.0000	0.7400	1.5090+08	0.3163	1.0000	2.9755-14
1.0000	0.7600	1.5090+08	0.2920	1.0000	2.9755-14
1.0000	0.7800	1.5090+08	0.2676	1.0000	2.9755-14
1.0000	0.8000	1.5090+08	0.2433	1.0000	2.9755-14
1.0000	0.8200	1.5090+08	0.2190	1.0000	2.9755-14
1.0000	0.8400	1.5090+08	0.1946	1.0000	2.9755-14
1.0000	0.8600	1.5090+08	0.1703	1.0000	2.9755-14
1.0000	0.8800	1.5090+08	0.1460	1.0000	2.9755-14
1.0000	0.9000	1.5090+08	0.1216	1.0000	2.9755-14
1.0000	0.9200	1.5090+08	9.7318-02	1.0000	2.9755-14
1.0000	0.9400	1.5090+08	7.2988-02	1.0000	2.9755-14
1.0000	0.9600	1.5090+08	4.8659-02	1.0000	2.9755-14
1.0000	0.9800	1.5090+08	2.4329-02	1.0000	2.9755-14
1.0000	1.0000	MISSING	1.0000	1.0000	0.0

FLASH CURVE TABLE: BINRY-1 (CONTINUED)

PRES ATM	MOLEFRAC WATER	MOLEFRAC LIQUID 1 WATER	MOLEFRAC LIQUID 1 TRIOL-01	MOLEFRAC LIQUID 2 WATER	MOLEFRAC LIQUID 2 TRIOL-01
1.0000	0.0	0.0	1.0000	MISSING	MISSING
1.0000	2.0000-02	2.0000-02	0.9800	MISSING	MISSING
1.0000	4.0000-02	4.0000-02	0.9600	MISSING	MISSING
1.0000	6.0000-02	6.0000-02	0.9400	MISSING	MISSING
1.0000	8.0000-02	8.0000-02	0.9200	MISSING	MISSING
1.0000	0.1000	0.1000	0.9000	MISSING	MISSING
1.0000	0.1200	0.1200	0.8800	MISSING	MISSING
1.0000	0.1400	0.1400	0.8600	MISSING	MISSING
1.0000	0.1600	0.1600	0.8400	MISSING	MISSING
1.0000	0.1800	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.2000	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.2200	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.2400	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.2600	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.2800	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.3000	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.3200	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.3400	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.3600	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.3800	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.4000	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.4200	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.4400	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.4600	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.4800	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.5000	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.5200	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.5400	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.5600	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.5800	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.6000	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.6200	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.6400	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.6600	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.6800	0.1780	0.8220	1.0000	1.9719-22

FLASH CURVE TABLE: BINRY-1 (CONTINUED)

PRES ATM	MOLEFRAC WATER	MOLEFRAC LIQUID 1 WATER	MOLEFRAC LIQUID 1 TRIOL-01	MOLEFRAC LIQUID 2 WATER	MOLEFRAC LIQUID 2 TRIOL-01
1.0000	0.7000	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.7200	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.7400	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.7600	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.7800	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.8000	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.8200	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.8400	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.8600	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.8800	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.9000	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.9200	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.9400	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.9600	0.1780	0.8220	1.0000	1.9719-22
1.0000	0.9800	0.1780	0.8220	1.0000	1.9719-22
1.0000	1.0000	1.0000	0.0	MISSING	MISSING

FLASH CURVE TABLE: BINRY-2

PROPERTIES ALONG A FLASH CURVE FOR THE MIXTURE: (KMOL/SEC   )
WATER   1.000   , METHANOL 1.000   ,

STATE SPECIFICATIONS:
VAPOR FRACTION: 0.000

VARIED VARIABLE(S):   PRES   MOLEFRAC

PROPERTY SET(S): $PS-TXY

3 PHASE PV FLASHES WERE PERFORMED.

PROPERTY OPTION SET: UNIFAC   UNIFAC / REDLICH-KWONG

FLASH CURVE TABLE: BINRY-2 (CONTINUED)

PRES ATM	MOLEFRAC WATER	TEMP TOTAL C	KVL TOTAL WATER	KVL TOTAL METHANOL	GAMMA LIQUID 1 WATER
1.0000	0.0	64.5348	0.4051	1.0000	1.6628
1.0000	2.0000-02	64.8429	0.4054	1.0121	1.6413
1.0000	4.0000-02	65.1533	0.4057	1.0248	1.6201
1.0000	6.0000-02	65.4661	0.4061	1.0379	1.5992
1.0000	8.0000-02	65.7813	0.4065	1.0516	1.5785
1.0000	0.1000	66.0990	0.4069	1.0659	1.5581
1.0000	0.1200	66.4194	0.4074	1.0808	1.5381
1.0000	0.1400	66.7426	0.4079	1.0964	1.5182
1.0000	0.1600	67.0687	0.4085	1.1127	1.4987
1.0000	0.1800	67.3978	0.4091	1.1297	1.4795
1.0000	0.2000	67.7302	0.4098	1.1475	1.4605
1.0000	0.2200	68.0660	0.4106	1.1663	1.4418
1.0000	0.2400	68.4053	0.4114	1.1859	1.4235
1.0000	0.2600	68.7485	0.4122	1.2065	1.4054
1.0000	0.2800	69.0958	0.4132	1.2282	1.3876
1.0000	0.3000	69.4474	0.4143	1.2510	1.3701
1.0000	0.3200	69.8036	0.4154	1.2751	1.3529
1.0000	0.3400	70.1648	0.4166	1.3005	1.3360
1.0000	0.3600	70.5314	0.4180	1.3274	1.3194
1.0000	0.3800	70.9037	0.4195	1.3558	1.3032
1.0000	0.4000	71.2823	0.4211	1.3859	1.2872
1.0000	0.4200	71.6676	0.4229	1.4179	1.2715
1.0000	0.4400	72.0604	0.4248	1.4519	1.2562
1.0000	0.4600	72.4612	0.4269	1.4882	1.2412
1.0000	0.4800	72.8708	0.4293	1.5268	1.2265
1.0000	0.5000	73.2902	0.4318	1.5682	1.2122
1.0000	0.5200	73.7203	0.4346	1.6125	1.1982
1.0000	0.5400	74.1623	0.4377	1.6601	1.1845
1.0000	0.5600	74.6174	0.4411	1.7113	1.1712
1.0000	0.5800	75.0874	0.4448	1.7666	1.1583
1.0000	0.6000	75.5738	0.4490	1.8265	1.1457
1.0000	0.6200	76.0788	0.4536	1.8915	1.1335
1.0000	0.6400	76.6047	0.4587	1.9622	1.1217
1.0000	0.6600	77.1544	0.4645	2.0395	1.1104
1.0000	0.6800	77.7312	0.4709	2.1244	1.0994

FLASH CURVE TABLE: BINRY-2 (CONTINUED)

PRES ATM	MOLEFRAC WATER	TEMP TOTAL C	KVL TOTAL WATER	KVL TOTAL METHANOL	GAMMA LIQUID 1 WATER
1.0000	0.7000	78.3390	0.4781	2.2178	1.0889
1.0000	0.7200	78.9825	0.4862	2.3212	1.0788
1.0000	0.7400	79.6673	0.4954	2.4361	1.0692
1.0000	0.7600	80.4001	0.5059	2.5647	1.0601
1.0000	0.7800	81.1892	0.5179	2.7093	1.0514
1.0000	0.8000	82.0448	0.5317	2.8730	1.0434
1.0000	0.8200	82.9792	0.5478	3.0600	1.0358
1.0000	0.8400	84.0082	0.5666	3.2751	1.0289
1.0000	0.8600	85.1517	0.5889	3.5253	1.0226
1.0000	0.8800	86.4349	0.6155	3.8194	1.0170
1.0000	0.9000	87.8911	0.6478	4.1696	1.0121
1.0000	0.9200	89.5640	0.6875	4.5933	1.0079
1.0000	0.9400	91.5127	0.7373	5.1149	1.0045
1.0000	0.9600	93.8189	0.8012	5.7713	1.0021
1.0000	0.9800	96.5980	0.8853	6.6189	1.0005
1.0000	1.0000	100.0178	1.0000	7.7494	1.0000

PRES ATM	MOLEFRAC WATER	GAMMA LIQUID 1 METHANOL	GAMMA LIQUID 2 WATER	GAMMA LIQUID 2 METHANOL	KVL2 TOTAL WATER
1.0000	0.0	1.0000	MISSING	MISSING	MISSING
1.0000	2.0000-02	1.0001	MISSING	MISSING	MISSING
1.0000	4.0000-02	1.0005	MISSING	MISSING	MISSING
1.0000	6.0000-02	1.0012	MISSING	MISSING	MISSING
1.0000	8.0000-02	1.0022	MISSING	MISSING	MISSING
1.0000	0.1000	1.0035	MISSING	MISSING	MISSING
1.0000	0.1200	1.0052	MISSING	MISSING	MISSING
1.0000	0.1400	1.0072	MISSING	MISSING	MISSING
1.0000	0.1600	1.0095	MISSING	MISSING	MISSING
1.0000	0.1800	1.0122	MISSING	MISSING	MISSING

FLASH CURVE TABLE: BINRY-2 (CONTINUED)

PRES ATM	MOLEFRAC WATER	GAMMA LIQUID 1 METHANOL	GAMMA LIQUID 2 WATER	GAMMA LIQUID 2 METHANOL	KVL2 TOTAL WATER
1.0000	0.2000	1.0153	MISSING	MISSING	MISSING
1.0000	0.2200	1.0189	MISSING	MISSING	MISSING
1.0000	0.2400	1.0228	MISSING	MISSING	MISSING
1.0000	0.2600	1.0273	MISSING	MISSING	MISSING
1.0000	0.2800	1.0322	MISSING	MISSING	MISSING
1.0000	0.3000	1.0376	MISSING	MISSING	MISSING
1.0000	0.3200	1.0436	MISSING	MISSING	MISSING
1.0000	0.3400	1.0502	MISSING	MISSING	MISSING
1.0000	0.3600	1.0573	MISSING	MISSING	MISSING
1.0000	0.3800	1.0652	MISSING	MISSING	MISSING
1.0000	0.4000	1.0737	MISSING	MISSING	MISSING
1.0000	0.4200	1.0830	MISSING	MISSING	MISSING
1.0000	0.4400	1.0931	MISSING	MISSING	MISSING
1.0000	0.4600	1.1040	MISSING	MISSING	MISSING
1.0000	0.4800	1.1158	MISSING	MISSING	MISSING
1.0000	0.5000	1.1287	MISSING	MISSING	MISSING
1.0000	0.5200	1.1426	MISSING	MISSING	MISSING
1.0000	0.5400	1.1576	MISSING	MISSING	MISSING
1.0000	0.5600	1.1739	MISSING	MISSING	MISSING
1.0000	0.5800	1.1915	MISSING	MISSING	MISSING
1.0000	0.6000	1.2105	MISSING	MISSING	MISSING
1.0000	0.6200	1.2311	MISSING	MISSING	MISSING
1.0000	0.6400	1.2535	MISSING	MISSING	MISSING
1.0000	0.6600	1.2777	MISSING	MISSING	MISSING
1.0000	0.6800	1.3039	MISSING	MISSING	MISSING
1.0000	0.7000	1.3325	MISSING	MISSING	MISSING
1.0000	0.7200	1.3635	MISSING	MISSING	MISSING
1.0000	0.7400	1.3972	MISSING	MISSING	MISSING
1.0000	0.7600	1.4339	MISSING	MISSING	MISSING
1.0000	0.7800	1.4741	MISSING	MISSING	MISSING
1.0000	0.8000	1.5179	MISSING	MISSING	MISSING
1.0000	0.8200	1.5659	MISSING	MISSING	MISSING
1.0000	0.8400	1.6185	MISSING	MISSING	MISSING
1.0000	0.8600	1.6764	MISSING	MISSING	MISSING
1.0000	0.8800	1.7401	MISSING	MISSING	MISSING

FLASH CURVE TABLE: BINRY-2 (CONTINUED)

PRES ATM	MOLEFRAC WATER	GAMMA LIQUID 1 METHANOL	GAMMA LIQUID 2 WATER	GAMMA LIQUID 2 METHANOL	KVL2 TOTAL WATER
1.0000	0.9000	1.8105	MISSING	MISSING	MISSING
1.0000	0.9200	1.8883	MISSING	MISSING	MISSING
1.0000	0.9400	1.9745	MISSING	MISSING	MISSING
1.0000	0.9600	2.0702	MISSING	MISSING	MISSING
1.0000	0.9800	2.1767	MISSING	MISSING	MISSING
1.0000	1.0000	2.2953	MISSING	MISSING	MISSING

PRES ATM	MOLEFRAC WATER	KVL2 TOTAL METHANOL	BETA TOTAL	MOLEFRAC VAPOR WATER	MOLEFRAC VAPOR METHANOL
1.0000	0.0	MISSING	1.0000	0.0	1.0000
1.0000	2.0000-02	MISSING	1.0000	8.1083-03	0.9919
1.0000	4.0000-02	MISSING	1.0000	1.6230-02	0.9838
1.0000	6.0000-02	MISSING	1.0000	2.4367-02	0.9756
1.0000	8.0000-02	MISSING	1.0000	3.2521-02	0.9675
1.0000	0.1000	MISSING	1.0000	4.0695-02	0.9593
1.0000	0.1200	MISSING	1.0000	4.8891-02	0.9511
1.0000	0.1400	MISSING	1.0000	5.7113-02	0.9429
1.0000	0.1600	MISSING	1.0000	6.5363-02	0.9346
1.0000	0.1800	MISSING	1.0000	7.3645-02	0.9264
1.0000	0.2000	MISSING	1.0000	8.1964-02	0.9180
1.0000	0.2200	MISSING	1.0000	9.0323-02	0.9097
1.0000	0.2400	MISSING	1.0000	9.8728-02	0.9013
1.0000	0.2600	MISSING	1.0000	0.1072	0.8928
1.0000	0.2800	MISSING	1.0000	0.1157	0.8843
1.0000	0.3000	MISSING	1.0000	0.1243	0.8757
1.0000	0.3200	MISSING	1.0000	0.1329	0.8671
1.0000	0.3400	MISSING	1.0000	0.1417	0.8583
1.0000	0.3600	MISSING	1.0000	0.1505	0.8495
1.0000	0.3800	MISSING	1.0000	0.1594	0.8406

FLASH CURVE TABLE: BINRY-2 (CONTINUED)

PRES ATM	MOLEFRAC WATER	KVL2 TOTAL METHANOL	BETA TOTAL	MOLEFRAC VAPOR WATER	MOLEFRAC VAPOR METHANOL
1.0000	0.4000	MISSING	1.0000	0.1684	0.8316
1.0000	0.4200	MISSING	1.0000	0.1776	0.8224
1.0000	0.4400	MISSING	1.0000	0.1869	0.8131
1.0000	0.4600	MISSING	1.0000	0.1964	0.8036
1.0000	0.4800	MISSING	1.0000	0.2060	0.7940
1.0000	0.5000	MISSING	1.0000	0.2159	0.7841
1.0000	0.5200	MISSING	1.0000	0.2260	0.7740
1.0000	0.5400	MISSING	1.0000	0.2364	0.7636
1.0000	0.5600	MISSING	1.0000	0.2470	0.7530
1.0000	0.5800	MISSING	1.0000	0.2580	0.7420
1.0000	0.6000	MISSING	1.0000	0.2694	0.7306
1.0000	0.6200	MISSING	1.0000	0.2812	0.7188
1.0000	0.6400	MISSING	1.0000	0.2936	0.7064
1.0000	0.6600	MISSING	1.0000	0.3066	0.6934
1.0000	0.6800	MISSING	1.0000	0.3202	0.6798
1.0000	0.7000	MISSING	1.0000	0.3347	0.6653
1.0000	0.7200	MISSING	1.0000	0.3501	0.6499
1.0000	0.7400	MISSING	1.0000	0.3666	0.6334
1.0000	0.7600	MISSING	1.0000	0.3845	0.6155
1.0000	0.7800	MISSING	1.0000	0.4040	0.5960
1.0000	0.8000	MISSING	1.0000	0.4254	0.5746
1.0000	0.8200	MISSING	1.0000	0.4492	0.5508
1.0000	0.8400	MISSING	1.0000	0.4760	0.5240
1.0000	0.8600	MISSING	1.0000	0.5065	0.4935
1.0000	0.8800	MISSING	1.0000	0.5417	0.4583
1.0000	0.9000	MISSING	1.0000	0.5830	0.4170
1.0000	0.9200	MISSING	1.0000	0.6325	0.3675
1.0000	0.9400	MISSING	1.0000	0.6931	0.3069
1.0000	0.9600	MISSING	1.0000	0.7691	0.2309
1.0000	0.9800	MISSING	1.0000	0.8676	0.1324
1.0000	1.0000	MISSING	1.0000	1.0000	0.0

FLASH CURVE TABLE: BINRY-2 (CONTINUED)

PRES ATM	MOLEFRAC WATER	MOLEFRAC LIQUID 1 WATER	MOLEFRAC LIQUID 1 METHANOL	MOLEFRAC LIQUID 2 WATER	MOLEFRAC LIQUID 2 METHANOL
1.0000	0.0	0.0	1.0000	MISSING	MISSING
1.0000	2.0000-02	2.0000-02	0.9800	MISSING	MISSING
1.0000	4.0000-02	4.0000-02	0.9600	MISSING	MISSING
1.0000	6.0000-02	6.0000-02	0.9400	MISSING	MISSING
1.0000	8.0000-02	8.0000-02	0.9200	MISSING	MISSING
1.0000	0.1000	0.1000	0.9000	MISSING	MISSING
1.0000	0.1200	0.1200	0.8800	MISSING	MISSING
1.0000	0.1400	0.1400	0.8600	MISSING	MISSING
1.0000	0.1600	0.1600	0.8400	MISSING	MISSING
1.0000	0.1800	0.1800	0.8200	MISSING	MISSING
1.0000	0.2000	0.2000	0.8000	MISSING	MISSING
1.0000	0.2200	0.2200	0.7800	MISSING	MISSING
1.0000	0.2400	0.2400	0.7600	MISSING	MISSING
1.0000	0.2600	0.2600	0.7400	MISSING	MISSING
1.0000	0.2800	0.2800	0.7200	MISSING	MISSING
1.0000	0.3000	0.3000	0.7000	MISSING	MISSING
1.0000	0.3200	0.3200	0.6800	MISSING	MISSING
1.0000	0.3400	0.3400	0.6600	MISSING	MISSING
1.0000	0.3600	0.3600	0.6400	MISSING	MISSING
1.0000	0.3800	0.3800	0.6200	MISSING	MISSING
1.0000	0.4000	0.4000	0.6000	MISSING	MISSING
1.0000	0.4200	0.4200	0.5800	MISSING	MISSING
1.0000	0.4400	0.4400	0.5600	MISSING	MISSING
1.0000	0.4600	0.4600	0.5400	MISSING	MISSING
1.0000	0.4800	0.4800	0.5200	MISSING	MISSING
1.0000	0.5000	0.5000	0.5000	MISSING	MISSING
1.0000	0.5200	0.5200	0.4800	MISSING	MISSING
1.0000	0.5400	0.5400	0.4600	MISSING	MISSING
1.0000	0.5600	0.5600	0.4400	MISSING	MISSING
1.0000	0.5800	0.5800	0.4200	MISSING	MISSING
1.0000	0.6000	0.6000	0.4000	MISSING	MISSING
1.0000	0.6200	0.6200	0.3800	MISSING	MISSING
1.0000	0.6400	0.6400	0.3600	MISSING	MISSING
1.0000	0.6600	0.6600	0.3400	MISSING	MISSING
1.0000	0.6800	0.6800	0.3200	MISSING	MISSING

FLASH CURVE TABLE: BINRY-2 (CONTINUED)

PRES ATM	MOLEFRAC WATER	MOLEFRAC LIQUID 1 WATER	MOLEFRAC LIQUID 1 METHANOL	MOLEFRAC LIQUID 2 WATER	MOLEFRAC LIQUID 2 METHANOL
1.0000	0.7000	0.7000	0.3000	MISSING	MISSING
1.0000	0.7200	0.7200	0.2800	MISSING	MISSING
1.0000	0.7400	0.7400	0.2600	MISSING	MISSING
1.0000	0.7600	0.7600	0.2400	MISSING	MISSING
1.0000	0.7800	0.7800	0.2200	MISSING	MISSING
1.0000	0.8000	0.8000	0.2000	MISSING	MISSING
1.0000	0.8200	0.8200	0.1800	MISSING	MISSING
1.0000	0.8400	0.8400	0.1600	MISSING	MISSING
1.0000	0.8600	0.8600	0.1400	MISSING	MISSING
1.0000	0.8800	0.8800	0.1200	MISSING	MISSING
1.0000	0.9000	0.9000	0.1000	MISSING	MISSING
1.0000	0.9200	0.9200	8.0000-02	MISSING	MISSING
1.0000	0.9400	0.9400	6.0000-02	MISSING	MISSING
1.0000	0.9600	0.9600	4.0000-02	MISSING	MISSING
1.0000	0.9800	0.9800	2.0000-02	MISSING	MISSING
1.0000	1.0000	1.0000	0.0	MISSING	MISSING

BLOCK STATUS

```
***************************************************************************
*                                                                         *
* Calculations were completed normally                                    *
*                                                                         *
* All Unit Operation blocks were completed normally                       *
*                                                                         *
* All streams were flashed normally                                       *
*                                                                         *
* All Property Tables were completed normally                             *
*                                                                         *
***************************************************************************
***************************************************************************
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;
;Input Summary created by Aspen Plus Rel. 39.0 at 01:06:38 Mon Apr 18, 2022
;Directory \\nestor\apadman\  Filename C:\Users\apadman\AppData\Local\Temp\~apa697.txt
;


DYNAMICS
   DYNAMICS RESULTS=ON

TITLE 'PHA Separation Train'

IN-UNITS SI PRESSURE=atm TEMPERATURE=C PDROP='N/sqm'

DEF-STREAMS CONVEN ALL

MODEL-OPTION

DESCRIPTION "


   "

DATABANKS 'APV121 POLYMER' / 'APV121 SEGMENT' / 'APV121 PURE37' &
        / 'APV121 INITIATO' / NOASPENPCD

PROP-SOURCES 'APV121 POLYMER' / 'APV121 SEGMENT' /  &
       'APV121 PURE37' / 'APV121 INITIATO'

COMPONENTS
   WATER H2O /
   METHANOL CH4O /
   CHLOR-01 CHCL3 /
   TRIOL-01 C57H104O6

SOLVE
   RUN-MODE MODE=SIM

FLOWSHEET
   BLOCK T400 IN=FEED OUT=METH WATER
   BLOCK T401 IN=FEED2 OUT=CHLORO TRIOL

PROPERTIES UNIFAC
   PROPERTIES SRK

STREAM FEED
   SUBSTREAM MIXED TEMP=25. PRES=1. MASS-FLOW=363122. <kg/hr>
   MASS-FLOW WATER 202748.0402 <kg/hr> / METHANOL  &
      160373.6998 <kg/hr>

STREAM FEED2
   SUBSTREAM MIXED TEMP=25.00000000 PRES=1.000000000  &
      MASS-FLOW=132509. <kg/hr>
   MASS-FLOW CHLOR-01 132029.5238 <kg/hr> / TRIOL-01  &
      479.1 <kg/hr>

BLOCK T400 RADFRAC
   SUBOBJECTS INTERNALS = CS-1
   PARAM NSTAGE=30 ALGORITHM=STANDARD HYDRAULIC=NO MAXOL=25  &
      DAMPING=NONE
   PARAM2 STATIC-DP=YES
   COL-CONFIG CONDENSER=TOTAL CA-CONFIG=INT-1
   FEEDS FEED 15
```

```
   PRODUCTS METH 1 L / WATER 30 L
   P-SPEC 1 1.
   COL-SPECS MASS-D:F=0.442 DP-STAGE=0. <atm> MOLE-RR=1.
   REPORT NOHYDRAULIC
   INTERNALS CS-1 STAGE1=2 STAGE2=29 P-UPDATE=NO  &
      TRAYTYPE=SIEVE NPASS=2 TRAY-SPACE=1.5 <ft>  &
      SYSFAC=1.000000000 OVER-DESIGN=1.000000000  &
      WEIR-HT=.0381000000 <meter> DC-CLEAR=.0254000000 <meter>  &
      DC-WTOP-SIDE=.8376809869 <meter>  &
      DC-WTOP-CTR=.6768107407 <meter>  &
      DC-WBOT-SIDE=.8376809869 <meter>  &
      DC-WBOT-CTR=.6768107407 <meter>  &
      HOLE-DIAM=.0127000000 <meter> HOLE-AREA=.1000000000  &
      FLOOD-METH=GLITSCH6 DECK-THICK=0.134 <IN>  &
      PCT-FLOOD-FA=80.00000000 AER-PARAM-M=1.000000000  &
      MAX-DC-LOAD=GLITSCH MAX-ACC-DP=2500.000000  &
      MAX-PCT-DCB=100.0000000 MAX-PCT-ENT=10.00000000  &
      MIN-WEIR-LD=1.24194040E-3 MAX-WEIR-LD=.0184278862  &
      MIN-PCT-DCA=.1000000000
   TRAY-SIZE 1 2 29 SIEVE

BLOCK T401 RADFRAC
   SUBOBJECTS INTERNALS = CS-1
   PARAM NSTAGE=15 ALGORITHM=STANDARD HYDRAULIC=NO MAXOL=25  &
      DAMPING=NONE
   PARAM2 STATIC-DP=YES OLD-SULZER=NO
   COL-CONFIG CONDENSER=TOTAL CA-CONFIG=INT-1
   FEEDS FEED2 7
   PRODUCTS CHLORO 1 L / TRIOL 15 L
   P-SPEC 1 1.000000000
   COL-SPECS MASS-D:F=0.99628 MASS-RR=0.8
   REPORT NOHYDRAULIC
   INTERNALS CS-1 STAGE1=2 STAGE2=14 P-UPDATE=NO  &
      TRAYTYPE=SIEVE NPASS=1 TRAY-SPACE=1.5 <ft>  &
      SYSFAC=1.000000000 OVER-DESIGN=1.000000000  &
      WEIR-HT=.0381000000 <meter> DC-CLEAR=.0254000000 <meter>  &
      DC-WTOP-SIDE=.6605983068 <meter>  &
      DC-WBOT-SIDE=.6605983068 <meter>  &
      HOLE-DIAM=.0127000000 <meter> HOLE-AREA=.1000000000  &
      FLOOD-METH=GLITSCH6 DECK-THICK=0.134 <IN>  &
      PCT-FLOOD-FA=80.00000000 AER-PARAM-M=1.000000000  &
      MAX-DC-LOAD=GLITSCH MAX-ACC-DP=2500.000000  &
      MAX-PCT-DCB=100.0000000 MAX-PCT-ENT=10.00000000  &
      MIN-WEIR-LD=1.24194040E-3 MAX-WEIR-LD=.0184278862  &
      MIN-PCT-DCA=.1000000000
   TRAY-SIZE 1 2 14 SIEVE

EO-CONV-OPTI

STREAM-REPOR MOLEFLOW MASSFLOW

PROPERTY-REP PCES

PROP-TABLE BINRY-1 FLASHCURVE
   IN-UNITS SI PRESSURE=atm TEMPERATURE=C PDROP='N/sqm'
   PROPERTIES UNIFAC FREE-WATER=STEAM-TA SOLU-WATER=3  &
      TRUE-COMPS=YES
   MOLE-FLOW WATER 1 /  TRIOL-01  1
   STATE VFRAC=0.0
   ANALYSIS ANAL-TYPE=TXY
   VARY PRES
   RANGE LIST=1.000000000
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    VARY MOLEFRAC COMP=WATER
    RANGE VARVALUE=RANGE LOWER=0.0 UPPER=1.0 NPOINT=50
    PARAM NPHASE=3

PROP-TABLE BINRY-2 FLASHCURVE
    IN-UNITS SI PRESSURE=atm TEMPERATURE=C PDROP='N/sqm'
    PROPERTIES UNIFAC FREE-WATER=STEAM-TA SOLU-WATER=3  &
        TRUE-COMPS=YES
    MOLE-FLOW WATER 1 /  METHANOL  1
    STATE VFRAC=0.0
    ANALYSIS ANAL-TYPE=TXY
    VARY PRES
    RANGE LIST=1.000000000
    VARY MOLEFRAC COMP=WATER
    RANGE VARVALUE=RANGE LOWER=0.0 UPPER=1.0 NPOINT=50
    PARAM NPHASE=3
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Material Safety Data Sheets

MATERIAL SAFETY DATA SHEET

1. Substance and Source Identification

National Institute of Standards and Technolo gy
Standard Reference Materials Program
100 Bureau Drive, Stop 2300
Gaithersburg, Maryland 20899-2300

SRM Number: 3091
MSDS Number: 3091
SRM Name: Aroclors in Methanol

Date of Issue: 26 January 2012

Telephone: 301-975-2200
FAX: 301-926-4751
E-mail: SRMMSDS@nist.gov

Emergency Telephone ChemTrec:
1-800-424-9300 (North America)
+1-703-527-3887 (International)

Description: This Standard Reference Material (SRM) is a set of six different solutions of individual Aroclors in methanol. These solutions are 99.9 % Methanol. A unit of SRM 3091 consist of six 2-mL ampoules, each containing approximately 1.2 mL of each of the following SRM solutions: SRM 3081 Aroclor 1016 in Methanol; SRM 3082 Aroclor 1232 in Methanol; SRM 3083 Aroclor 1242 in Methanol; SRM 3084 Aroclor 1248 in Methanol; SRM 3085 Aroclor 1254 in Methanol; and SRM 3086 Aroclor 1260 in Methanol. This SRM is intended primarily for calibrating chromatographic instrumentation and methods of analysis used for the determination of Aroclors and polychlorinated byphenyls (PCBs) in water.

Substance: Methanol.

Other Designations: Wood alcohol; wood spirit; methyl hydroxide; methyl alcohol.

2. Hazards Identification

NFPA Ratings (Scale 0-4): Health = 2 Fire = 3 Reactivity = 0

NOTE: The health and safety information included in this MSDS is for methanol, the main component of this SRM. The concentration of Aroclors in this NIST SRM is below the reportable limits for hazardous components (1 %) and/or carcinogens (0.1 %), as required by OSHA, 29 CFR 1910.1200 (g)(2)(i)(C)(1), for MSDS information.

Major Health Hazards: Skin and eye irritation, central nervous system depression, and nerve damage.

Physical Hazards: Flammable liquid and vapor. Vapor may cause flash fire.

Potential Health Effects

Inhalation: Exposure may cause irritation of the mucous membranes, coughing, tracheitis, bronchitis, tinnitus, unsteady gait, twitching, constipation, nystagmus, and blepharospams. Repeated exposure may result in recurrent headaches, diminution of vision, enlargement of the liver, and allergic reactions.

Skin Contact: Exposure may cause irritation. Skin absorption may occur and cause metabolic acidosis and effect on the eyes and central nervous system. Repeated or long-term exposure may lead to defatting of the skin resulting in erythema, scaling, and eczematoid dermatitis.

Eye Contact: Vapors may cause irritation. High concentrations have been reported to cause violent inflammation of the conjunctiva and epithelial defects on the cornea. Repeated or prolonged contact may cause conjunctivitis.

Ingestion: Ingestion may result in mild and transient inebriation and subsequent drowsiness followed by an asymptomatic period lasting 8-48 hours. Following the delay, coughing, dyspnea, headache, dullness, weakness, nausea, vomiting, violent pain in the back, abdomen, and extremities, apathy or delirium may occur. Rapid shallow respiration due to metabolic acidosis, hypotension, cyanosis, convulsions, cardiac depression, cerebral and pulmonary edema, unconsciousness, and coma may occur. Liver, kidney, heart, stomach, intestine and pancreatic damage may also occur. Death may occur due to respiratory failure. As little as 15 mL has caused blindness; the usual fatal dose is 60–240 mL.

Listed as a Carcinogen/Potential Carcinogen

	Yes	No
In the National Toxicology Program (NTP) Report on Carcinogens		X
In the International Agency Report on Carcinogens (IARC) Monographs		X
By the Occupational Safety and Health Administration (OSHA)		X

3. COMPOSITION AND INFORMATION ON HAZARDOUS INGREDIENTS

Component[a]	CAS Registry	EC Number (EINECS)	Nominal Concentration
Methanol	67-56-1	200-659-6	>99.9 %

[a] This material is a complex mixture that has not been tested as a whole. The material contains organic compounds (see Certificate of Analysis), which have been reported to have toxic, mutagenic, and/or carcinogenic properties, and should be handled with care. Components are listed in accordance with OSHA, 29 CFR 1910.1200 (g)(2)(i)(C)(1) which requires identification of hazardous components at concentrations greater than 1 % and carcinogens at concentrations greater than 0.1 %.

EC Classification: T, F
EC Risk (R No.): 11, 39/23/24/25
EC Safety (S No.): 7, 16, 36/37, 45

EC Risk/Safety Phrases: Refer to Section 15, "Regulatory Information".

Note: EC information is based on the concentration of methanol in solution. The listed EC information is for a methanol solution of 10 % or greater.

4. FIRST AID MEASURES

Inhalation: If adverse effects occur, remove to uncontaminated area. If not breathing, give artificial respiration or oxygen by qualified personnel. Seek immediate medical attention.

Eye Contact: Immediately flush eyes, including under the eyelids with copious amounts of water for at least 15 minutes. Seek immediate medical attention.

Skin Contact: Rinse affected area with copious amounts of water followed by washing with soap and water for at least 15 minutes while removing contaminated clothing. Seek medical attention, if needed.

Ingestion: Contact a poison control center immediately for instructions. Give water to rinse out mouth. Never give liquids to a person with reduced awareness or becoming unconscious. If vomiting occurs, keep head lower than hips to prevent aspiration. If not breathing, give artificial respiration by qualified personnel. Seek immediate medical attention.

5. FIRE FIGHTING MEASURES

Fire and Explosion Hazards: Severe fire hazard. Vapor/air mixtures are explosive. The vapor is heavier than air. Vapors or gases may ignite at distant ignition sources and flash back. OSHA Class IB flammable liquid.

Extinguishing Media: Alcohol-resistant foam, carbon dioxide, regular dry chemical, water.

Fire Fighting: Avoid inhalation of material or combustion byproducts. Wear full protective clothing and NIOSH-approved self-contained breathing apparatus (SCBA).

Flash Point: 11 ºC (52 ºF)
Method Used: Closed Cup

Autoignition Temp: 385 ºC (725 ºF)

Flammability Limits in Air
UPPER (Volume %): 36
LOWER (Volume %): 6

6. ACCIDENTAL RELEASE MEASURES

Occupational Release: Avoid heat, flames, sparks and other sources of ignition. Do not touch spilled material. Stop leak if possible without personal risk. Reduce vapors with water spray. Absorb small spills with sand or other non-combustible material. Collect spilled material in appropriate container for disposal. Remove sources of ignition. Keep unnecessary people away, isolate hazard area and deny entry.

Disposal: Refer to Section 13, "Disposal Considerations".

7. HANDLING AND STORAGE

Handling and Storage: Store and handle in accordance with all current regulations and standards. Ampoules should be stored at room temperature. Subject to storage regulations: U.S. OSHA 29 CFR 1910.106. Grounding and bonding required. Keep separated from incompatible substances.

Safe Handling Precautions: See Section 8, "Exposure Controls and Personal Protection".

8. Exposure Controls and Personal Protection

Exposure Limits:

ACGIH (TWA): 200 ppm
ACGIH (STEL): 250 ppm
ACGIH: Skin – potential significant contribution to overall exposure by the cutaneous route
OSHA (TWA): 200 ppm, 260 mg/m^3
NIOSH (TWA): 200 ppm; 260 mg/m^3
NIOSH (STEL): 250 ppm; 325 mg/m^3
NIOSH (IDLH): 6000 ppm
NIOSH: Potential for dermal absorption.

Ventilation: Use local exhaust ventilation system. Ensure compliance with applicable exposure limits. Refer to the ACGIH document, *Industrial Ventilation, a Manual of Recommended Practices*.

Respirator: If workplace conditions warrant a respirator, a respiratory protection program that meets OSHA 29 CFR 1910.134 must be followed. Refer to NIOSH 42 CFR 84 for applicable certified respirators.

Eye Protection: Wear chemical safety goggles. An eyewash station should be readily available near areas of use.

Personal Protection: Wear appropriate protective clothing and chemically resistant gloves to prevent skin exposure.

9. Physical and Chemical Properties

Appearance and Odor: Colorless liquid, alcohol odor

Odor Threshold: 100 ppm

Molar Mass (g/mol): 32.04

Molecular Formula: CH_3OH

Melting Point: –94 ºC (–137 ºF)

Boiling Point: 65 ºC (149 ºF)

Vapor Pressure: 97.25 mmHg at 20 ºC

Vapor Density (air = 1): 1.11

Specific Gravity (water = 1): 0.7914

Water Solubility: Soluble

10. Stability and Reactivity

Stability: __X__ Stable _____ Unstable

Stable at normal temperatures and pressure.

Conditions to Avoid: Avoid heat, flames, sparks, and other sources of ignition.

Incompatible Materials: Halogens, oxidizing materials, combustible materials, metals, bases, and acids.

Fire/Explosion Information: See Section 5, "Fire Fighting Measures".

Hazardous Decomposition: Oxides of carbon and miscellaneous decomposition products.

Hazardous Polymerization: _____ Will Occur __X__ Will Not Occur

11. Toxicological Information

Route of Entry: X Inhalation X Skin X Ingestion

Toxicity Data:

Rat, Oral LC_{50}: 5628 mg/kg
Rat, Inhalation LC_{50}: 83.2 mg/L (4 h)
Rabbit, Skin LD_{50}: 5600 mg/kg
Rabbit, Eyes (Irritation): 100 mg/24 hours, moderate.

Target Organ(s): Nervous system. May cause blindness

Health Effects (Acute and Chronic): See Section 2, "Hazards Identification" for potential health effects.

Medical Conditions Aggravated by Exposure: Eye disorders, skin disorders, and kidney disorders.

Mutagenic, Reproductive, and Tumorigenic Toxic Effects: The components of this material have been reviewed and the Registry of Toxic Effects of Chemical Substances (RTECS) publishes the following endpoints.

Tumorigenic:	No data available.
Mutagenic:	Rat, Oral: 10 μmol/kg (DNA damage) Human, lymphocyte: 300 mmol/L (DNA inhibition)
Reproductive:	Rat, Inhalation TCLo: 20 000 ppm/7 h (pregnant, 1–22 d, Specific developmental abnormalities: musculoskeletal, cardiovascular, and urogenital system.)

12. Ecological Information

Ecotoxicity Data: Fish Toxicity: Fathead minnow (*Pimephales promelas*) LC_{50} (static): >100 mg/L (96 h)
Fish Toxicity: Steelhead trout (*Oncorhynchus mykiss*) LC_{50} (static): 18–20 mL/L (96 h)

13. Disposal Considerations

Waste Disposal: Dispose in accordance with all applicable federal, state, and local requirements. Subject to disposal regulations: U.S. EPA 40CFR 262.

14. Transportation Information

U.S. DOT and IATA: Methanol, Hazard Class 3 (6.1), UN1230, Packing Group II, Excepted Qty: Yes, E2.

15. Regulatory Information

U.S. REGULATIONS

CERCLA Sections 102a/103 (40 CFR 302.4): 5000 lb (2270 kg) final RQ.
SARA Title III Section 302 (40 CFR 355.30): Not regulated for this material.
SARA Title III Section 304 (40 CFR 355.40): Not regulated for this material.
SARA Title III Section 313 (40 CFR 372.65): 0.1 % de minimis concentration.
OSHA Process Safety (29 CFR 1910.119): Not regulated for this material.
SARA Title III Sections 311/312 Hazardous Categories (40 CFR 370.21):

ACUTE:	Yes
CHRONIC:	Yes
FIRE:	Yes
REACTIVE:	No
SUDDEN RELEASE:	No

STATE REGULATIONS

California Proposition 65: Not listed.

CANADIAN REGULATIONS

WHMIS Classification: Not provided for this material.

EUROPEAN REGULATIONS

EC Classification:
F: Flammable
T: Toxic

EC Risk Phrases:
R11 – Highly flammable.
R39/23/24/25 – Toxic: Danger of very serious irreversible effects through inhalation, in contact with skin and if swallowed.

EC Safety Phrases:
S7 – Keep container tightly closed.
S16 – Keep away from sources of ignition – No smoking.
S36/37 – Wear suitable protective clothing and gloves.
S45 – In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible).

NATIONAL INVENTORY STATUS

U.S. Inventory (TSCA): Listed.

TSCA 12(b)
Export Notification: Not listed.

16. OTHER INFORMATION

Sources: ChemAdvisor, Inc., MSDS *Methyl Alcohol*, 20 December 2011.

EC; European Chemical Substance Information System (ESIS), *Methanol*, CAS No. 67-56-1; available at http://esis.jrc.ec.europa.eu/ (accessed Jan 2012).

NIOSH Registry of Toxic Effects of Chemical Substances (RTECS), *Methanol, No. PC1400000, CAS No. 67-56-1*; May 2009; available at http://www.cdc.gov/niosh-rtecs/PC155CC0.html (accessed Jan 2012).

Chloroform

Safety Data Sheet

according to Federal Register / Vol. 77, No. 58 / Monday, March 26, 2012 / Rules and Regulations
Date of issue: 06/03/2013 Revision date: 03/21/2017 Supersedes: 03/21/2017 Version: 1.3

SECTION 1: Identification

1.1. Identification

Product form	:	Substance
Substance name	:	Chloroform
CAS-No.	:	67-66-3
Product code	:	LC13040
Formula	:	CHCl3
Synonyms	:	1,1,1-trichloromethane / Chloroform / formyl trichloride / freon 20 / methane trichloride / methane, trichloro- / methenyl chloride / methenyl trichloride / methyl trichloride / R 20 / R 20 refrigerant / TCM (=trichloromethane) / trichloroform / trichloromethane

1.2. Recommended use and restrictions on use

Use of the substance/mixture	:	Bactericide Fumigant Insecticide Solvent Chemical substance for research
Recommended use	:	Laboratory chemicals
Restrictions on use	:	Not for food, drug or household use

1.3. Supplier

LabChem, Inc.

Jackson's Pointe Commerce Park Building 1000, 1010 Jackson's Pointe Court

Zelienople, PA 16063 - USA

T 412-826-5230 - F 724-473-0647

1.4. Emergency telephone number

Emergency number	:	CHEMTREC: 1-800-424-9300 or +1-703-741-5970

SECTION 2: Hazard(s) identification

2.1. Classification of the substance or mixture

GHS-US classification

Acute toxicity (oral) Category 4	H302	Harmful if swallowed
Acute toxicity (inhalation) Category 3	H331	Toxic if inhaled
Skin corrosion/irritation Category 2	H315	Causes skin irritation
Serious eye damage/eye irritation Category 2A	H319	Causes serious eye irritation
Carcinogenicity Category 2	H351	Suspected of causing cancer
Reproductive toxicity Category 2	H361	Suspected of damaging the unborn child.
Specific target organ toxicity (repeated exposure) Category 1	H372	Causes damage to organs (liver, kidneys) through prolonged or repeated exposure (Inhalation, oral)

Full text of H statements : see section 16

2.2. GHS Label elements, including precautionary statements

GHS US labeling

Hazard pictograms (GHS US) :

GHS06 GHS07 GHS08

Signal word (GHS US)	:	Danger
Hazard statements (GHS US)	:	H302 - Harmful if swallowed H315 - Causes skin irritation

H319 - Causes serious eye irritation
H331 - Toxic if inhaled
H351 - Suspected of causing cancer
H361 - Suspected of damaging the unborn child.
H372 - Causes damage to organs (liver, kidneys) through prolonged or repeated exposure (Inhalation, oral)

Precautionary statements (GHS US) : P201 - Obtain special instructions before use.
P202 - Do not handle until all safety precautions have been read and understood.
P260 - Do not breathe vapors.
P264 - Wash exposed skin thoroughly after handling.
P270 - Do not eat, drink or smoke when using this product.
P271 - Use only outdoors or in a well-ventilated area.
P280 - Wear eye protection, face protection, protective clothing, protective gloves.
P301+P312 - IF SWALLOWED: Call a POISON CENTER or doctor/physician if you feel unwell.
P302+P352 - IF ON SKIN: Wash with plenty of soap and water.
P304+P340 - IF INHALED: Remove person to fresh air and keep comfortable for breathing.
P305+P351+P338 - If in eyes: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing
P308+P313 - IF exposed or concerned: Get medical advice/attention.
P311 - Call a POISON CENTER or doctor/physician.
P330 - If swallowed, rinse mouth
P332+P313 - If skin irritation occurs: Get medical advice/attention.
P337+P313 - If eye irritation persists: Get medical advice/attention.
P362+P364 - Take off contaminated clothing and wash it before reuse.
P403+P233 - Store in a well-ventilated place. Keep container tightly closed.
P405 - Store locked up.
P501 - Dispose of contents/container to comply with local, state and federal regulations

2.3. Other hazards which do not result in classification

Other hazards not contributing to the classification : None.

2.4. Unknown acute toxicity (GHS US)

Not applicable

SECTION 3: Composition/Information on ingredients

3.1. Substances

Substance type : Multi-constituent

Name	Product identifier	%	GHS-US classification
Chloroform (Main constituent)	(CAS-No.) 67-66-3	99	Acute Tox. 4 (Oral), H302 Acute Tox. 3 (Inhalation), H331 Skin Irrit. 2, H315 Eye Irrit. 2A, H319 Carc. 2, H351 Repr. 2, H361 STOT RE 1, H372
Ethanol (Distributor)	(CAS-No.) 64-17-5	1	Flam. Liq. 2, H225 Carc. 1A, H350 Repr. 2, H361

Full text of hazard classes and H-statements : see section 16

3.2. Mixtures

Not applicable

SECTION 4: First-aid measures

4.1. Description of first aid measures

First-aid measures general : Check the vital functions. Unconscious: maintain adequate airway and respiration. Respiratory arrest: artificial respiration or oxygen. Cardiac arrest: perform resuscitation. Victim conscious with labored breathing: half-seated. Victim in shock: on his back with legs slightly raised. Vomiting: prevent asphyxia/aspiration pneumonia. Prevent cooling by covering the victim (no warming up). Keep watching the victim. Give psychological aid. Keep the victim calm, avoid physical strain. Depending on the victim's condition: doctor/hospital. Never give alcohol to drink.

First-aid measures after inhalation : Remove the victim into fresh air. Respiratory problems: consult a doctor/medical service.

First-aid measures after skin contact : Wash immediately with lots of water. Soap may be used. Do not apply (chemical) neutralizing agents. Take victim to a doctor if irritation persists.

First-aid measures after eye contact : Rinse immediately with plenty of water. Do not apply neutralizing agents. Take victim to an ophthalmologist if irritation persists.

First-aid measures after ingestion	: Rinse mouth with water. Immediately after ingestion: give lots of water to drink. Do not give milk/oil to drink. Do not induce vomiting. Call Poison Information Centre (www.big.be/antigif.htm). Consult a doctor/medical service if you feel unwell. Ingestion of large quantities: immediately to hospital. Take the container/vomit to the doctor/hospital.

4.2. Most important symptoms and effects (acute and delayed)

Symptoms/effects after inhalation	: Feeling of weakness. Dry/sore throat. Central nervous system depression. Headache. Nausea. Vomiting. Dizziness. Narcosis. Mental confusion. Drunkenness. Coordination disorders. Disturbances of consciousness. Disturbances of heart rate. Enlargement/affection of the liver. Affection of the renal tissue.
Symptoms/effects after skin contact	: Red skin. Dry skin. Tingling/irritation of the skin. ON CONTINUOUS EXPOSURE/CONTACT: Blisters.
Symptoms/effects after eye contact	: Irritation of the eye tissue.
Symptoms/effects after ingestion	: Risk of aspiration pneumonia. Irritation of the gastric/intestinal mucosa. Symptoms similar to those listed under inhalation.
Chronic symptoms	: ON CONTINUOUS/REPEATED EXPOSURE/CONTACT: Behavioural disturbances. Impaired concentration. Delusions. Gastrointestinal complaints. Degeneration of heart tissue. Enlargement/affection of the liver. Yellow skin. Affection of the renal tissue.

4.3. Immediate medical attention and special treatment, if necessary

Obtain medical assistance.

SECTION 5: Fire-fighting measures

5.1. Suitable (and unsuitable) extinguishing media

Suitable extinguishing media	: Adapt extinguishing media to the environment.
Unsuitable extinguishing media	: No unsuitable extinguishing media known.

5.2. Specific hazards arising from the chemical

Fire hazard	: DIRECT FIRE HAZARD. Non-flammable. INDIRECT FIRE HAZARD. May build up electrostatic charges: risk of ignition. Reactions involving a fire hazard: see "Reactivity Hazard".
Explosion hazard	: INDIRECT EXPLOSION HAZARD. Reactions with explosion hazards: see "Reactivity Hazard".
Reactivity	: Violent to explosive reaction with many compounds: release of heat. Decomposes slowly on exposure to light and on exposure to air: release of toxic and corrosive gases/vapours (phosgene, chlorine, hydrogen chloride). Reacts with (strong) oxidizers: release of toxic and corrosive gases/vapours (phosgene, chlorine).

5.3. Special protective equipment and precautions for fire-fighters

Precautionary measures fire	: Exposure to fire/heat: consider evacuation.
Firefighting instructions	: Cool tanks/drums with water spray/remove them into safety. Do not move the load if exposed to heat. Dilute toxic gases with water spray. Take account of toxic/corrosive precipitation water.
Protection during firefighting	: Do not enter fire area without proper protective equipment, including respiratory protection.

SECTION 6: Accidental release measures

6.1. Personal precautions, protective equipment and emergency procedures

6.1.1. For non-emergency personnel

Protective equipment	: Gloves. Protective goggles. Head/neck protection. Protective clothing. Large spills/in enclosed spaces: gas-tight suit. Reactivity hazard: gas-tight suit. See "Material-Handling" to select protective clothing.
Emergency procedures	: Keep upwind. Mark the danger area. Seal off low-lying areas. Close doors and windows of adjacent premises. No naked flames. Keep containers closed. Protect substance against light. Wash contaminated clothes. Large spills/in confined spaces: consider evacuation. In case of reactivity hazard: consider evacuation.

6.1.2. For emergency responders

Protective equipment	: Equip cleanup crew with proper protection.
Emergency procedures	: Stop leak if safe to do so. Ventilate area.

6.2. Environmental precautions

Prevent spreading in sewers.

6.3. Methods and material for containment and cleaning up

For containment : Contain released substance, pump into suitable containers. Consult "Material-handling" to select material of containers. Plug the leak, cut off the supply. Dam up the liquid spill. Try to reduce evaporation. Provide equipment/receptacles with earthing. Dilute narcotic gases/vapours with water spray. If reacting: dilute toxic gas/vapour with water spray. Take account of toxic/corrosive precipitation water.

Methods for cleaning up : Take up liquid spill into inert absorbent material, e.g.: sand, earth, vermiculite. Scoop absorbed substance into closing containers. See "Material-handling" for suitable container materials. Carefully collect the spill/leftovers. Clean contaminated surfaces with an excess of water. Take collected spill to manufacturer/competent authority. Wash clothing and equipment after handling.

6.4. Reference to other sections

No additional information available

SECTION 7: Handling and storage

7.1. Precautions for safe handling

Precautions for safe handling : Comply with the legal requirements. Remove contaminated clothing immediately. Clean contaminated clothing. Thoroughly clean/dry the installation before use. Do not discharge the waste into the drain. Use earthed equipment. Keep away from naked flames/heat. Observe strict hygiene. Keep container tightly closed. Measure the concentration in the air regularly. Carry operations in the open/under local exhaust/ventilation or with respiratory protection.

Hygiene measures : Wash hands and other exposed areas with mild soap and water before eating, drinking or smoking and when leaving work. Wash contaminated clothing before reuse.

7.2. Conditions for safe storage, including any incompatibilities

Storage conditions : Keep container tightly closed.

Heat-ignition : KEEP SUBSTANCE AWAY FROM: heat sources.

Prohibitions on mixed storage : KEEP SUBSTANCE AWAY FROM: oxidizing agents. strong acids. (strong) bases.

Storage area : Store in a dark area. Ventilation at floor level. Fireproof storeroom. Provide for a tub to collect spills. Provide the tank with earthing. Unauthorized persons are not admitted. Store only in a limited quantity. Meet the legal requirements. Store at ambient temperature.

Special rules on packaging : SPECIAL REQUIREMENTS: hermetical. clean. opaque. correctly labelled. meet the legal requirements. Secure fragile packagings in solid containers.

Packaging materials : SUITABLE MATERIAL: metal. steel. stainless steel. iron. glass. tin. MATERIAL TO AVOID: aluminium. copper.

SECTION 8: Exposure controls/personal protection

8.1. Control parameters

Chloroform (67-66-3)		
ACGIH	ACGIH TWA (ppm)	10 ppm (Chloroform; USA; Time-weighted average exposure limit 8 h; TLV - Adopted Value)
NIOSH	NIOSH REL (STEL) (mg/m³)	9.78 mg/m³ 60 min.
NIOSH	NIOSH REL (STEL) (ppm)	2 ppm 60 min.

Ethanol (64-17-5)		
ACGIH	ACGIH STEL (ppm)	1000 ppm
NIOSH	NIOSH REL (TWA) (mg/m³)	1900 mg/m³
NIOSH	NIOSH REL (TWA) (ppm)	1000 ppm

8.2. Appropriate engineering controls

Appropriate engineering controls : Emergency eye wash fountains should be available in the immediate vicinity of any potential exposure.

8.3. Individual protection measures/Personal protective equipment

Personal protective equipment:

Gas mask. Gloves. Safety glasses.

Materials for protective clothing:

GIVE EXCELLENT RESISTANCE: PVA. viton. GIVE GOOD RESISTANCE: No data available. GIVE LESS RESISTANCE: chlorinated polyethylene. neoprene. nitrile rubber. polyethylene. neoprene/natural rubber. nitrile rubber/PVC. GIVE POOR RESISTANCE: butyl rubber. natural rubber. PVC. styrene-butadiene rubber. neoprene/SBR

Hand protection:

Gloves

Eye protection:

Safety glasses

Skin and body protection:

Head/neck protection. Protective clothing

Respiratory protection:

Gas mask with filter type AX at conc. in air > exposure limit. High vapour/gas concentration: self-contained respirator

SECTION 9: Physical and chemical properties

9.1. Information on basic physical and chemical properties

Physical state	: Liquid
Appearance	: Liquid.
	: Colourless
	: Sweet odour Ether-like odour
Odor threshold	: 133 - 276 ppm 648 - 1344 mg/m³
pH	: No data available
Melting point	: -64 °C
Freezing point	: No data available
Boiling point	: 61 °C
Critical temperature	: 263 °C
Critical pressure	: 54702 hPa
Flash point	: No data available
Relative evaporation rate (butyl acetate=1)	: 11.6
Relative evaporation rate (ether=1)	: 1.9
Flammability (solid, gas)	: No data available
Vapor pressure	: 209.5 hPa (20 °C)
Relative vapor density at 20 °C	: 4.1
Relative density	: 1.49 (20 °C)
Relative density of saturated gas/air mixture	: 1.7
Specific gravity / density	: 1490 kg/m³ (20 °C)
Molecular mass	: 119.38 g/mol

Solubility	:	Poorly soluble in water. Substance sinks in water. Soluble in ethanol. Soluble in ether. Soluble in acetone. Soluble in oil. Soluble in carbondisulfide. Soluble in petroleum spirit. Soluble in naphtha. Soluble in tetrachloromethane. Water: 0.87 g/100ml (23 °C, poorly soluble) Ethanol: soluble Ether: soluble Acetone: soluble
Log Pow	:	1.97 (Experimental value; 20 °C)
Auto-ignition temperature	:	> 600 °C (1013 hPa)
Decomposition temperature	:	No data available
Viscosity, kinematic	:	No data available
Viscosity, dynamic	:	No data available
Explosion limits	:	No data available
Explosive properties	:	No data available
Oxidizing properties	:	No data available

9.2. Other information

Specific conductivity	:	< 10000 pS/m
Saturation concentration	:	1045 g/m³
VOC content	:	100 %
Other properties	:	Gas/vapour heavier than air at 20°C. Clear. Volatile. No data available. May generate electrostatic charges.

SECTION 10: Stability and reactivity

10.1. Reactivity

Violent to explosive reaction with many compounds: release of heat. Decomposes slowly on exposure to light and on exposure to air: release of toxic and corrosive gases/vapours (phosgene, chlorine, hydrogen chloride). Reacts with (strong) oxidizers: release of toxic and corrosive gases/vapours (phosgene, chlorine).

10.2. Chemical stability

Unstable on exposure to light. Unstable on exposure to air.

10.3. Possibility of hazardous reactions

No additional information available

10.4. Conditions to avoid

Direct sunlight. Air contact.

10.5. Incompatible materials

No additional information available

10.6. Hazardous decomposition products

Chlorine.

SECTION 11: Toxicological information

11.1. Information on toxicological effects

Likely routes of exposure	:	Inhalation; Skin and eye contact
Acute toxicity	:	Not classified

Chloroform (67-66-3)	
LD50 oral rat	695 mg/kg (Rat; OECD 401: Acute Oral Toxicity; Experimental value; 908 mg/kg bodyweight; Rat; OECD 401: Acute Oral Toxicity; Experimental value; 1117 mg/kg bodyweight; Rat)
LD50 dermal rabbit	> 20000 mg/kg (Rabbit; No reliable data available; >3980 mg/kg bodyweight; Rabbit)
ATE US (oral)	695 mg/kg body weight
ATE US (gases)	700 ppmV/4h
ATE US (vapors)	3 mg/l/4h
ATE US (dust, mist)	0.5 mg/l/4h

Ethanol (64-17-5)	
LD50 oral rat	10740 mg/kg (Rat; Experimental value,Rat; Experimental value)
LD50 dermal rabbit	> 16000 mg/kg (Rabbit, Literature study, Dermal)

Ethanol (64-17-5)	
LC50 inhalation rat (mg/l)	117 - 125 mg/l air (Equivalent or similar to OECD 403, 4 h, Rat, Male / female, Experimental value, Inhalation)
ATE US (oral)	10740 mg/kg body weight

Skin corrosion/irritation : Causes skin irritation.

Serious eye damage/irritation : Causes serious eye irritation.

Respiratory or skin sensitization : Not classified

Germ cell mutagenicity : Not classified

Carcinogenicity : Suspected of causing cancer.

Chloroform (67-66-3)	
IARC group	2B - Possibly carcinogenic to humans

Chloroform (67-66-3)	
IARC group	2B - Possibly carcinogenic to humans

Reproductive toxicity : Suspected of damaging the unborn child.

Specific target organ toxicity – single exposure : Not classified

Specific target organ toxicity – repeated exposure : Causes damage to organs (liver, kidneys) through prolonged or repeated exposure (Inhalation, oral).

Aspiration hazard : Not classified

Symptoms/effects after inhalation : Feeling of weakness. Dry/sore throat. Central nervous system depression. Headache. Nausea. Vomiting. Dizziness. Narcosis. Mental confusion. Drunkenness. Coordination disorders. Disturbances of consciousness. Disturbances of heart rate. Enlargement/affection of the liver. Affection of the renal tissue.

Symptoms/effects after skin contact : Red skin. Dry skin. Tingling/irritation of the skin. ON CONTINUOUS EXPOSURE/CONTACT: Blisters.

Symptoms/effects after eye contact : Irritation of the eye tissue.

Symptoms/effects after ingestion : Risk of aspiration pneumonia. Irritation of the gastric/intestinal mucosa. Symptoms similar to those listed under inhalation.

Chronic symptoms : ON CONTINUOUS/REPEATED EXPOSURE/CONTACT: Behavioural disturbances. Impaired concentration. Delusions. Gastrointestinal complaints. Degeneration of heart tissue. Enlargement/affection of the liver. Yellow skin. Affection of the renal tissue.

SECTION 12: Ecological information

12.1. Toxicity

Ecology - general : Not classified as dangerous for the environment according to the criteria of Regulation (EC) No 1272/2008.

Ecology - air : Not classified as dangerous for the ozone layer (Regulation (EC) No 1005/2009). Not included in the list of substances which may contribute to the greenhouse effect (Regulation (EC) No 842/2006). TA-Luft Klasse 5.2.5/I.

Ecology - water : Groundwater pollutant. Harmful to fishes. Harmful to invertebrates (Daphnia). Harmful to algae.

Chloroform (67-66-3)	
LC50 fish 1	18.2 ppm (LC50; ASTM; 96 h; Oncorhynchus mykiss; Flow-through system; Fresh water; Experimental value)
EC50 Daphnia 2	152.5 mg/l (EC50; US EPA; 48 h; Daphnia magna; Static system; Salt water; Experimental value)

Ethanol (64-17-5)	
LC50 fish 1	14200 mg/l (US EPA, 96 h, Pimephales promelas, Flow-through system, Fresh water, Experimental value)

12.2. Persistence and degradability

Chloroform (67-66-3)	
Persistence and degradability	Not readily biodegradable in water. Non degradable in the soil. Low potential for adsorption in soil.
ThOD	0.33 - 1.35 g O_2/g substance
BOD (% of ThOD)	0.015 - 0.06

Ethanol (64-17-5)	
Persistence and degradability	Biodegradable in the soil. Readily biodegradable in water.
Biochemical oxygen demand (BOD)	0.8 - 0.967 g O_2/g substance
Chemical oxygen demand (COD)	1.7 g O_2/g substance
ThOD	2.1 g O_2/g substance
BOD (% of ThOD)	0.43

12.3. Bioaccumulative potential

Chloroform (67-66-3)	
BCF fish 2	1.4 - 4.7 (BCF; OECD 305: Bioconcentration: Flow-Through Fish Test; 42 days; Cyprinus carpio; Flow-through system; Fresh water; Experimental value)
Log Pow	1.97 (Experimental value; 20 °C)
Bioaccumulative potential	Low potential for bioaccumulation (BCF < 500).
Ethanol (64-17-5)	
BCF fish 1	1 (Other, 72 h, Cyprinus carpio, Static system, Fresh water, Read-across)
Log Pow	-0.31 (Experimental value)
Bioaccumulative potential	Not bioaccumulative.

12.4. Mobility in soil

Chloroform (67-66-3)	
Surface tension	0.0271 N/m (20 °C)
Log Koc	Koc,Other; 86.7-367; Experimental value; log Koc; Other; 1.94-2.56; Experimental value
Ecology - soil	May be harmful to plant growth, blooming and fruit formation.
Ethanol (64-17-5)	
Surface tension	0.022 N/m (20 °C)
Ecology - soil	Highly mobile in soil.

12.5. Other adverse effects

No additional information available

SECTION 13: Disposal considerations

13.1. Disposal methods

Waste disposal recommendations	: Remove waste in accordance with local and/or national regulations. Hazardous waste shall not be mixed together with other waste. Different types of hazardous waste shall not be mixed together if this may entail a risk of pollution or create problems for the further management of the waste. Hazardous waste shall be managed responsibly. All entities that store, transport or handle hazardous waste shall take the necessary measures to prevent risks of pollution or damage to people or animals. Recycle by distillation. Dissolve or mix with a combustible solvent. Remove to an incinerator for chlorinated waste materials with energy recovery. Do not discharge into drains or the environment. Do not discharge into surface water (Directive 2000/60/EC, Council Decision 2455/2001/EC).
Additional information	: LWCA (the Netherlands): KGA category 04. Hazardous waste according to Directive 2008/98/EC.
Ecology - waste materials	: Avoid release to the environment.

SECTION 14: Transport information

Department of Transportation (DOT)

In accordance with DOT

Transport document description	: UN1888 Chloroform, 6.1, III
UN-No.(DOT)	: UN1888
Proper Shipping Name (DOT)	: Chloroform
Packing group (DOT)	: III - Minor Danger

Hazard labels (DOT)	: 6.1 - Poison

DOT Packaging Non Bulk (49 CFR 173.xxx)	: 203
DOT Packaging Bulk (49 CFR 173.xxx)	: 241
DOT Special Provisions (49 CFR 172.102)	: IB3 - Authorized IBCs: Metal (31A, 31B and 31N); Rigid plastics (31H1 and 31H2); Composite (31HZ1 and 31HA2, 31HB2, 31HN2, 31HD2 and 31HH2). Additional Requirement: Only liquids with a vapor pressure less than or equal to 110 kPa at 50 C (1.1 bar at 122 F), or 130 kPa at 55 C (1.3 bar at 131 F) are authorized, except for UN2672 (also see Special Provision IP8 in Table 2 for UN2672). N36 - Aluminum or aluminum alloy construction materials are permitted only for halogenated hydrocarbons that will not react with aluminum. T7 - 4 178.274(d)(2) Normal............ 178.275(d)(3) TP2 - a. The maximum degree of filling must not exceed the degree of filling determined by the following: (image) Where: tr is the maximum mean bulk temperature during transport, tf is the temperature in degrees celsius of the liquid during filling, and a is the mean coefficient of cubical expansion of the liquid between the mean temperature of the liquid during filling (tf) and the maximum mean bulk temperature during transportation (tr) both in degrees celsius. b. For liquids transported under ambient conditions may be calculated using the formula: (image) Where: d15 and d50 are the densities (in units of mass per unit volume) of the liquid at 15 C (59 F) and 50 C (122 F), respectively.
DOT Packaging Exceptions (49 CFR 173.xxx)	: 153
DOT Quantity Limitations Passenger aircraft/rail (49 CFR 173.27)	: 60 L
DOT Quantity Limitations Cargo aircraft only (49 CFR 175.75)	: 220 L
DOT Vessel Stowage Location	: A - The material may be stowed ''on deck'' or ''under deck'' on a cargo vessel and on a passenger vessel.
DOT Vessel Stowage Other	: 40 - Stow ''clear of living quarters''
Other information	: No supplementary information available.

Transportation of Dangerous Goods

Transport document description	: UN1888 CHLOROFORM, 6.1, III
UN-No. (TDG)	: UN1888
Proper Shipping Name (Transportation of Dangerous Goods)	: CHLOROFORM
TDG Primary Hazard Classes	: 6.1 - Class 6.1 - Toxic Substances
Packing group	: III - Minor Danger
Explosive Limit and Limited Quantity Index	: 5 L
Passenger Carrying Road Vehicle or Passenger Carrying Railway Vehicle Index	: 60 L

Transport by sea

Transport document description (IMDG)	: UN 1888 , 6.1, III
UN-No. (IMDG)	: 1888
Class (IMDG)	: 6.1 - Toxic substances
Packing group (IMDG)	: III - substances presenting low danger
EmS-No. (1)	: F-A
EmS-No. (2)	: S-A

Air transport

Transport document description (IATA)	: UN 1888 , 6.1, III
UN-No. (IATA)	: 1888
Class (IATA)	: 6 -
Packing group (IATA)	: III - Minor Danger

SECTION 15: Regulatory information

15.1. US Federal regulations

Chloroform (67-66-3)	
Listed on the United States TSCA (Toxic Substances Control Act) inventory Subject to reporting requirements of United States SARA Section 313	
RQ (Reportable quantity, section 304 of EPA's List of Lists)	10 lb
SARA Section 311/312 Hazard Classes	Health hazard - Acute toxicity (any route of exposure) Health hazard - Carcinogenicity Health hazard - Reproductive toxicity Health hazard - Serious eye damage or eye irritation Health hazard - Skin corrosion or Irritation Health hazard - Specific target organ toxicity (single or repeated exposure)
SARA Section 313 - Emission Reporting	0.1 %

All components of this product are listed, or excluded from listing, on the United States Environmental Protection Agency Toxic Substances Control Act (TSCA) inventory

Chemical(s) subject to the reporting requirements of Section 313 or Title III of the Superfund Amendments and Reauthorization Act (SARA) of 1986 and 40 CFR Part 372.

Chloroform	CAS-No. 67-66-3	99%

Chloroform (67-66-3)	
RQ (Reportable quantity, section 304 of EPA's List of Lists)	10 lb
SARA Section 311/312 Hazard Classes	Health hazard - Acute toxicity (any route of exposure) Health hazard - Carcinogenicity Health hazard - Reproductive toxicity Health hazard - Serious eye damage or eye irritation Health hazard - Skin corrosion or Irritation Health hazard - Specific target organ toxicity (single or repeated exposure)
SARA Section 313 - Emission Reporting	0.1 %

15.2. International regulations

CANADA

Chloroform (67-66-3)
Listed on the Canadian DSL (Domestic Substances List)

Chloroform (67-66-3)
Listed on the Canadian DSL (Domestic Substances List)

EU-Regulations

No additional information available

National regulations

Chloroform (67-66-3)
Listed on the Canadian IDL (Ingredient Disclosure List)

Chloroform (67-66-3)
Listed on the Canadian IDL (Ingredient Disclosure List)

Ethanol (64-17-5)
Listed on IARC (International Agency for Research on Cancer)

15.3. US State regulations

Chloroform (67-66-3)	
U.S. - California - Proposition 65 - Carcinogens List	Yes
U.S. - California - Proposition 65 - Developmental Toxicity	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Female	No
U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No
No significant risk level (NSRL)	20 µg/day

This product can expose you to Chloroform, which is known to the State of California to cause cancer. For more information go to www.P65Warnings.ca.gov.

Chloroform (67-66-3)				
U.S. - California - Proposition 65 - Carcinogens List	U.S. - California - Proposition 65 - Developmental Toxicity	U.S. - California - Proposition 65 - Reproductive Toxicity - Female	U.S. - California - Proposition 65 - Reproductive Toxicity - Male	No significant risk level (NSRL)
Yes	No	No	No	20 µg/day

SECTION 16: Other information

Revision date : 03/21/2017

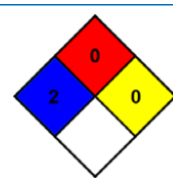
Full text of H-phrases: see section 16:

H225	Highly flammable liquid and vapour
H302	Harmful if swallowed
H315	Causes skin irritation
H319	Causes serious eye irritation
H331	Toxic if inhaled
H350	May cause cancer
H351	Suspected of causing cancer
H361	Suspected of damaging fertility or the unborn child
H372	Causes damage to organs through prolonged or repeated exposure

NFPA health hazard : 2 - Materials that, under emergency conditions, can cause temporary incapacitation or residual injury.

NFPA fire hazard : 0 - Materials that will not burn under typical fire conditions, including intrinsically noncombustible materials such as concrete, stone, and sand.

NFPA reactivity : 0 - Material that in themselves are normally stable, even under fire conditions.



Hazard Rating

Health : 2 Moderate Hazard - Temporary or minor injury may occur

Flammability : 0 Minimal Hazard - Materials that will not burn

Physical : 0 Minimal Hazard - Materials that are normally stable, even under fire conditions, and will NOT react with water, polymerize, decompose, condense, or self-react. Non-Explosives.

Personal protection : H

H - Splash goggles, Gloves, Synthetic apron, Vapor respirator